STRUCTURES AND MAGNETIC PROPERTIES OF POLYNUCLEAR COMPLEXES WITH AMINOALCOHOLS AND IMINOALCOHOLS AS LIGANDS

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STRUCTURES AND MAGNETIC PROPERTIES OF POLYNUCLEAR COMPLEXES WITH AMINOALCOHOLS AND IMINOALCOHOLS AS LIGANDS

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The author wishes to express her thanks to her husband, Ichiro, for his understanding and help.

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SUMMARY

The polynuclear complexes of transition metals with aminoalcohols and iminoalcohols studied can be classified, according to the type of bridging group present, as either hydrogen-bonded or as oxygen-bridged complexes.

The hydrogen-bonded dinuclear complex, (2-aminoethoxo)bis(2-aminoethonol)nickel(II) perchlolate was prepared and the structure was solved by X-ray diffraction. Two tris chelate complexes, each possessing threefold symmetry, are related by an inversion center. This structure exhibits a twofold disorder of the ligand positions, but the occupancy factors refined to values near 1/3 and 2/3. These values indicate four ligands of one type and two of another type for each dimeric unit. Considering the disorder, there are two short oxygen-oxygen distances indicative of edge-to-edge hydrogen-bonding. The room temperature magnetic moment of the complex, 3.16 BM per gram atom of nickel, is within the normal range for octahedral nickel(II) and the value at 93 °K is only slightly lower, 3.04 BM. Compounds of the formula $MM'(Eta)_n(EtaH)_{6-n}(ClO_4)_2$ (where M = Ni and M′ = Fe, Mn, Zn, Cr, and Co; and where M = Co and M′ = Fe, Mn, Mg, Zn, and Co) have been prepared and characterized by elemental analysis, X-ray diffraction, and magnetic moments. In these preparations, the metal atoms M and M′ are not present in exactly a 1:1 ratio, indicating impurities, the structures are isostructural to the nickel compound.

Several hydrogen-bonded dinuclear complexes, $Cu(L)(LH)X \cdot nH_2O$ (where L is the anion of 2-aminoethanol or a substituted 2-aminoethanol, X is ClO_4 or NO_3 and n is zero or one) have been synthesized and found to have similar structures. The bis-chelated planar copper complexes are associated into hydrogen-bonded dinuclear units in these compounds. The oxygen-oxygen distances of hydrogen-bonding range from 2.39Å to 2.52Å. All of these complexes show weak antiferromagnetic coupling. However, there is no simple correlation of the magnitude of antiferromagnetic coupling and either the oxygen-oxygen distances of the hydrogen bonds or any other identifiable structure feature.

The crystal structure of bis(2,2′-dioxodiethylamine) (2,2′-dihydroxydiethylamine)dicobalt(II,III) perchlorate has been studied by X-ray diffraction. The structure consists of tetrameric units linked by weak hydrogen bonds into zig-zag chains. The tetrameric unit has the same type of structure as the titanium alkoxides with two μ_3-alkoxide and four μ-alkoxide bridging atoms. The magnetic moments of this compound at various temperatures indicate weak antiferromagnetic coupling of the cobalt(II) atoms.

The crystal structure of bis[N-(picolinoyl)-3-amino-1-propoxoaquo-copper(II)] dihydrate has been studied by X-ray diffraction. The structure consists of dimeric units and waters of crystallization that are linked by weak hydrogen-bonding into infinite, nearly-planar networks. The dimeric unit has twofold symmetry and contains a bent Cu_2O_2 ring (dihedral angle of 15.8(4)° between the O-Cu-O planes). The magnetic susceptibility data previously reported for this compound were interpreted

as a weak magnetic coupling for which there was no exact fit to a polynuclear coupling equation. For this reason, two kinds of magnetic interactions within the cluster were predicted, but lack of structural information prohibited confirmation of the predictions. The X-ray structure analysis indicates that the weak antiferromagnetic coupling is due to a bent Cu_2O_2 four-membered ring and the discrepancy from the dimeric coupling equation might be the result of hydrogen bonding between dimeric units.

CHAPTER I

INTRODUCTION

Although a cobalt complex of 2-aminoethanol was isolated in 1932,[1] no systematic studies have been done on the resulting compound until very recently.[2] It is known that the aminoethanols are normally more acidic than diamines, and the aminoalkoxides that result from deprotonation show increased chelating tendency. The conditions of preparation (mainly the pH of the solution) and the properties of the metal ion determine whether alcohol or alkoxide groups of these ligands are coordinated to the metal. There is also a strong tendency for the coordinated alkoxide of a deprotonated aminoethanol to form polynuclear complexes by forming additional bonds with other metal atoms (oxygen bridges) or with protons of coordinated alcohol groups (hydrogen-bonded bridges). Several oxygen-bridged polynuclear complexes and hydrogen-bonded (O-H$\cdots$O bridged) dinuclear complexes have been isolated.

Polynuclear compounds containing unpaired electrons may exhibit ferromagnetic or antiferromagnetic behavior. A ferromagnetic substance shows normal paramagnetic behavior above a certain temperature, called the Curie temperature. Below the Curie temperature, the magnetic susceptibility of a ferromagnetic material is magnetic field-strength dependent and shows a temperature dependence different from that above the Curie temperature. For antiferromagnetism there is again a characteristic temperature, called the Néel temperature. Above the Néel temperature

the substance has the behavior of a simple paramagnetic substance, but below the Néel temperature the susceptibility decreases with decreasing temperature. Antiferromagnetic behavior may involve direct metal-metal bonding in some cases, but most examples of both antiferromagnetic and ferromagnetic behavior involve indirect interactions, or superexchanges through the bridging groups.

Because of widely varied structures and interesting magnetic properties, the transition metal complexes of aminoalcohols have recently received more attention. The purpose of this work is to reach a better understanding of the relationship between structural parameters and magnetic properties by systematically studying polynuclear complexes with aminoalcohols and iminoalcohols through synthesis, investigation of magnetic properties, and single crystal X-ray diffraction structure determination.

Mononuclear and polynuclear cobalt complexes of 2-aminoethanol (abbreviated EtaH) were first reported by W. Hieber and E. Levy.[1,3] $Co(EtaH)_3X_2$, $Co(Eta)(EtaH)_2X$, $Co_2(Eta)(EtaH)_5X_3$, and $Co_3(Eta)_4(EtaH)_2(H_2O)_2X_2$ (where X = Cl, Br, and I. Eta represents the anion of 2-aminoethanol. All abbreviations of ligands are listed in Table 1) were prepared and characterized as cobalt(II) complexes. Several mononuclear nickel, copper, and zinc complexes of 2-aminoethanol were also reported.[3]

H. Brintzinger and B. Hesse[4] reported $Co(Eta)_2(EtaH)\cdot 3H_2O$ and $Co_2(Eta)(EtaH)_5(NO_3)_3$ which were formulated as containing only cobalt(II).

Later, H. Yoneda and S. Kida[5] prepared complexes, $Co_2(Eta)_3(EtaH)_3(NO_3)_3$, $Co_2(Eta)_3(EtaH)_3Br_3\cdot 4H_2O$ and $Co(Eta)_3$ which were characterized

Table 1. Abbreviations Used for Ligands

Deta	the dianion of 2,2′-dihydroxydiethylamine
DiimH	the dianion of the diimine of 2,4-pentanedione and 2-aminoethanol
Dme	the anion of N,N′-dimethyl-2-aminoethanol
EIA	the dianion of the imine of 2,4-pentanedione and 2-aminoethanol
ℓ-Eph	the anion of ℓ-ephedrine, N-methyl-2-amino-1-phenyl-1-propanol
Eta	the anion of 2-aminoethanol
Mep	the anion of 2-amino-2-methylpropanol
PIA	the dianion of the imine of 2,4-pentanedione and 3-amino-1-propanol
PIPA	the dianion of N-picolinoyl-3-amino-1-propanol
PYPA	the dianion of the imine of pyrrole-2-carboxaldehyde and 3-amino-1-propanol
Teta	the anion of 2-aminoethanethiol

Table 2. Abbreviations Used for Compounds

NiNiEtaP	$[Ni(Eta)(EtaH)_2]_2(ClO_4)_2$
MM′EtaP	$MM'(Eta)_n(EtaH)_{6-n}(ClO_4)_2$
$Co^{II}Co^{II}$EtaP	$[Co(Eta)(EtaH)_2]_2(ClO_4)_2$
CoNiEtaI	$CoNi(Eta)_3(EtaH)_3I_2$
$Co^{III}Co^{III}$EtaP	$Co_2(Eta)_3(EtaH)_3(ClO_4)_3 \cdot 1/2\ H_2O$
Co-trimer	$Co_3(Eta)_6(OAc)_2$
CuEta	$[Cu(Eta)(EtaH)]_2(NO_3)_2$
CuMep	$[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$
Cu(ℓ-Eph)	$[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$
CuDme	$[Cu(Dme)(DmeH)]_2(ClO_4)_2$
CuDiimH	$[CuDiimH]_2$
CoDeta	$[Co_2(Deta)_2(DetaH_2)]_2(ClO_4)_2$

as cobalt(III) compounds. For the dinuclear cobalt(III) complexes, hydrogen-bonded cations were suggested and dinuclear structures containing octahedral tris chelates with one (corner-to-corner bonding shown in Figure 1) to three (face-to-face bonding shown in Figure 2) hydroben bonds were considered.

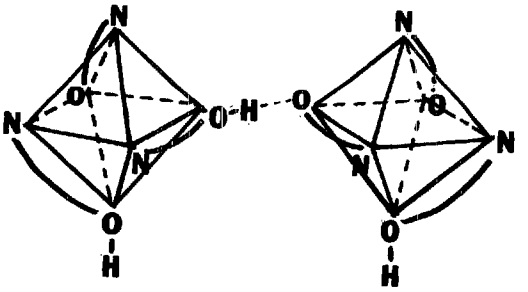


Figure 1. Corner-to-Corner Bonding

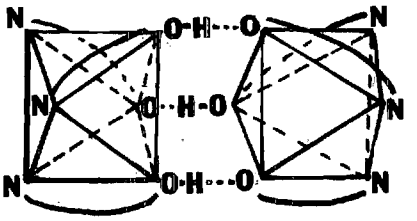


Figure 2. Face-to-Face Bonding

More recently V. V. Vdovenko and A. N. Gerasenkova reported a series of trinuclear complexes with the formula $[Co_3(Eta)_6]X_2 \cdot nH_2O$.[6,7] Potentiometric analyses for cobalt(II) and for total cobalt indicated one cobalt(II) and two cobalt(III) ions per formula unit. These workers proposed a structure with face-sharing octahedra. The structural study by J. A. Bertrand, J. A. Kelly, and E. G. Vassian[8] has confirmed both the face-sharing arrangement and the octahedral coordination of the terminal cobalt(III) atoms (Figure 3). The central cobalt(II), however, was found to be six coordinate with an almost perfect trigonal prismatic arrangement of alkoxide oxygens.

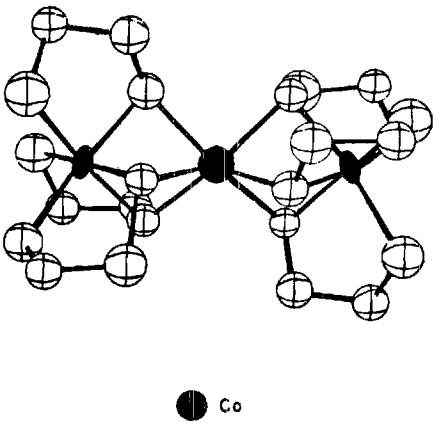


Figure 3. Structure of the Trinuclear Cobalt(II)-Cobalt(III) Complex of 2-Aminoethanol.

In preparing a series of complexes of various metal ions with tris-(2-aminoethoxo)cobalt(III) as ligands, a compound of composition $[CoNi(Eta)_3(EtaH)_3]I_2$ was isolated by J. A. Bertrand, W. J. Howard,

and A. R. Kalyanaraman.[9] Crystal structure analysis has shown a cubic crystal system, Pa3, with dimeric units of $\bar{3}$ symmetry (Figure 4). Two tris chelated complexes, each possessing threefold symmetry, are related by an inversion center. Two sets of ligand positions were located due to disorder and were assumed to correspond to chelate rings on the two different metal ions. The two sets of ligand positions, each with an occupancy factor of 0.5, were used in refining the structure. Although hydrogens were not located, the short oxygen-oxygen distance of 2.51Å and the stereochemistry at the oxygens indicated face-to-face hydrogen-bonding.

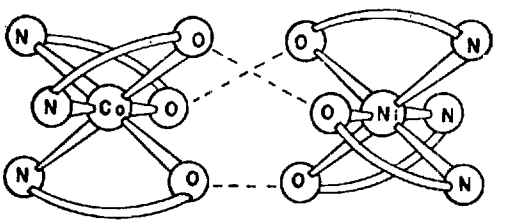


Figure 4. The Structure of the Dinuclear Hydrogen-bonded Cation, $[CoNi(Eta)_3(EtaH)_3]^{2+}$

Although mononuclear and/or polynuclear chromium,[3,4,10] zinc,[3] nickel,[3,11] and copper[3,11-13] complexes of 2-aminoethanol have been prepared, these complexes have not been well characterized. Also trinuclear mixed-metal complexes with the formula $MCo_2(Eta)_6X_2$ (where M = Co(II), Zn(II), Ni(II), Mg(II), and Cu(II)) have been isolated,[14-18] but systematic structural and magnetic studies of these complexes have

not been reported.

Recently, hydrogen-bonded dinuclear copper and nickel complexes with the diimine of 2-aminoethanol and 2,4-pentanedione (abbreviated $DiimH_3$ and shown in Figure 5) were reported.[19,20] Two crystallographically independent dimeric molecules in the unit cell showed almost identical bond distances and bond angles. The chelated copper(II) monomers of Cu(DiimH) were associated into hydrogen-bonded dinuclear units about inversion centers (Figure 6), and the resulting metal-metal distances are 4.989 and 4.987Å. The oxygen-oxygen distances between the ligands were only 2.31 and 2.33Å, and strong hydrogen bonding was suggested. The room temperature magnetic moment of 1.68 BM per atom of copper was below the spin only value of 1.73 BM, and the moment dropped to 1.56 BM at 193°K and 1.14 BM at 77°K. This behavior is characteristic of antiferromagnetic superexchange with a coupling constant, 2J, of -94 cm^{-1}.

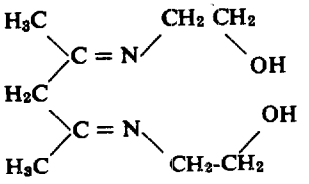


Figure 5. Diimine of 2-Aminoethanol and 2,4-Pentanedione, $DiimH_3$

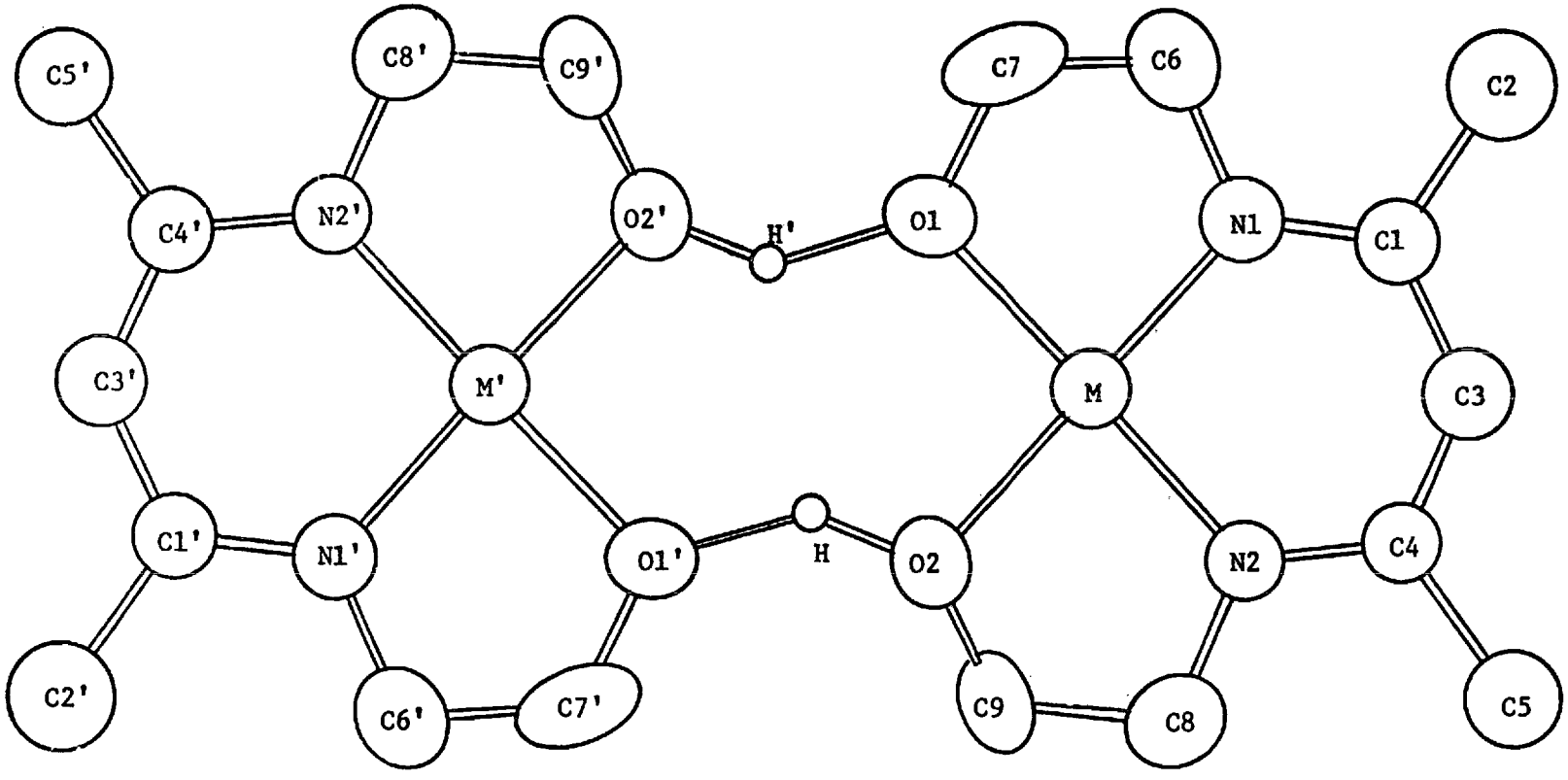


Figure 6. Structure of the Hydrogen-bonded Copper(II) Dimer of DiimH

Amano and coworkers[21,22] isolated and solved the structure of copper complex with ℓ-ephedrine (N-methyl-2-amino-1-phenylpropanol). This compound, $Cu(\ell\text{-Eph})_2 \cdot 2/3\ C_6H_6$, (where ℓ-Eph represents the anion of ℓ-ephedrine) had a trans square-planar coordination of copper (Figure 7). The molecular structure consisted of a triangular arrangement of square-planar copper complexes connected by oxygen-nitrogen hydrogen-bonding. The nitrogen-oxygen distance was 2.87Å and no measurement of magnetic coupling was reported.

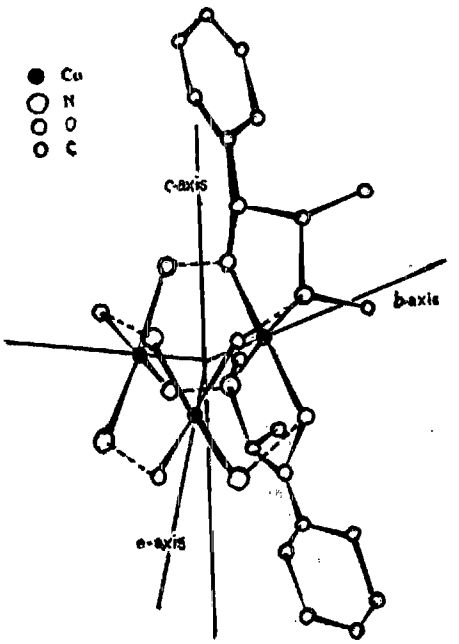


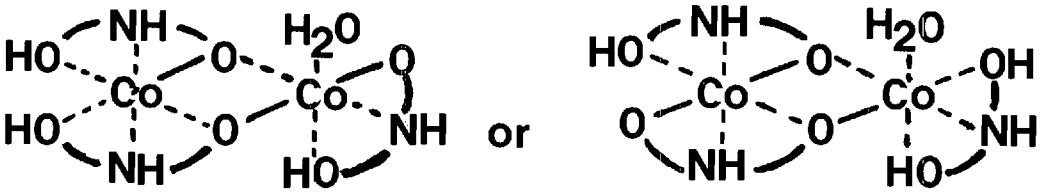
Figure 7. Structure of $[Cu(\ell\text{-Eph})_2]_3$

Dimer formation through intermolecular hydrogen-bonding is well documented for compounds such as carboxylic acids, but there have been

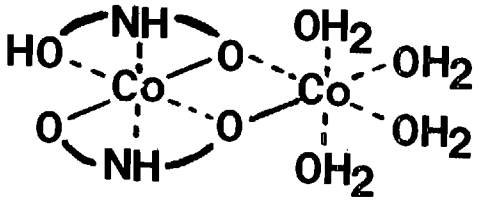
relatively few examples of hydrogen-bonded polynuclear transition metal complexes.[9,19,20,22,23] Although antiferromagnetic coupling was observed for $[Cu(DiimH)]_2$, the magnetic properties of most of the hydrogen-bonded complexes have not been studied. It would be interesting to compare the magnetic properties of hydrogen-bonded complexes of paramagnetic metal ions to determine the relationship between magnetic coupling and structures; such a comparison should lead to better understanding of the mechanism of superexchange. For this reason a systematic study of the preparation, structural analysis, and magnetic properties of hydrogen-bonded metal complexes of 2-aminoethanol and substituted 2-aminoethanol was initiated.

Interesting complexes of other aminoethanols have also been reported. Mononuclear and dinuclear cobalt complexes of 2,2′-dihydroxydiethylamine, $DetaH_2$, were first reported by W. Hieber and E. Levy in 1932.[3] $Co(DetaH_2)(OH)X$, $Co(DetaH)(H_2O)X$, $Co_2(DetaH)_3 - 3H](H_2O)X$, $Co_2(DetaH)(Deta)(H_2O)_4X$, and $Co_2(DetaH)(Deta)(H_2O)X$ (where X = Cl, Br, and I) were prepared and were reported as cobalt(II) compounds. The dimer structures they proposed are shown in Figure 3.

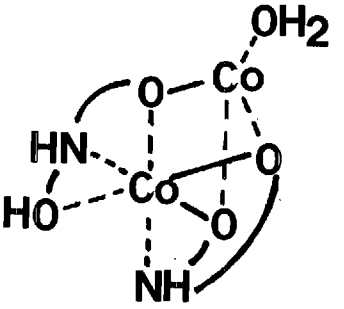
More recently two types of "dinuclear" cobalt complexes of 2,2′-dihydroxydiethylamine, $Co_2(Deta)_2(DetaH_2)X$, and $Co_2(Deta)_2X\cdot 4H_2O$ (where X = Cl, Br, and I) were prepared by V. N. Evreev and G. A. Kotlyar.[24] Potentiometric analysis for cobalt(II) and for total cobalt indicated that these complexes contained cobalt(II) and cobalt(III) in the ratio 1:1. A face-sharing octahedral dinuclear structure for $Co_2(Deta)_2(DetaH_2)X$ and a face-sharing or edge-sharing octahedral



$Co_2[(DetaH_2)_3 - 3H](H_2O)\ X$



$Co_2(DetaH)(Deta)(H_2O)_4X$



$Co_2(DetaH)(Deta)(H_2O)X$

Figure 8. Proposed Structures of Dinuclear Cobalt Complexes of 2,2′-Dihydroxydiethylamine

dinuclear structure for $Co_2(Deta)_2X\cdot 4H_2O$ were proposed. Three other similar complexes, $Co_2(Deta)_2(DetaH_2)\ ClO_4\cdot nH_2O$ (n = 1 and 3) and $Co_2(Deta)_2ClO_4\cdot 2H_2O$ [25] were also prepared. As a result of the treatment of these complexes in alkaline solution, complexes of the type $M[Co(Deta)_2]\cdot nH_2O$ (where M = Na and n = 8, and where M = K and n = 7) were isolated. Evreev and Golub[26] also proposed the existence of a trinuclear complex of the type $Co_3(Deta)_4\cdot nH_2O$, which was not isolated.

A polynuclear complex, $NaCo_6[(DetaH_2)_6 - 7H](OH)_4(CO_3)_3\cdot 12H_2O$ was prepared by A. Yao[27] and an attempt was made to solve the structure of this complex by X-ray diffraction. This complex contained cobalt(II) and cobalt(III) in the ratio 2:1. The crystallographic study revealed as a portion of the structure an arrangement of cobalt atoms similar to the tetrameric unit present in titanium alkoxides (Figure 9).[28-31] Due to twinning, disordered atoms and/or poor data, the remaining two cobalt atoms were not located.

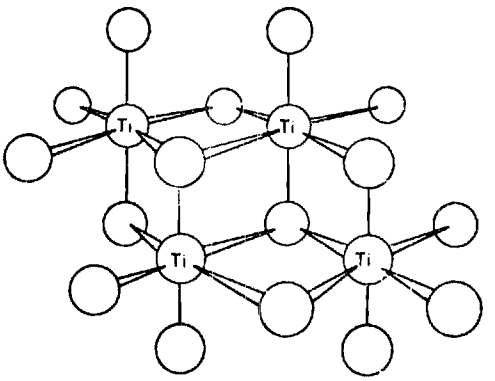


Figure 9. The Tetrameric Structure of Crystalline $Ti(OC_2H_5)_4$. Only Ti and O Atoms Are Shown.

Although cobalt complexes of 2,2′-dihydroxydiethylamine were isolated in 1932, neither complete crystal structures nor magnetic properties have been reported due to difficulties in obtaining good crystals. These compounds probably have oxygen-bridged structures, but further work is needed for an understanding of their structures and properties.

The tendency of the amine function to condense with carbonyl compounds makes possible a number of iminoalcohol ligands from amino-alcohols, and some of these form interesting polynuclear complexes. Recently, the preparation and properties of two copper(II) complexes containing the dianion of N-(picolinoyl)-3-amino-1-propanol (abbreviated PIPA and shown in Figure 10) were reported.[32,33] An anhydrous material with empirical formula CuPIPA was isolated and found to exhibit anti-ferromagnetic behavior. The magnetic susceptibility observed for this compound at temperatures above 150°K agreed well with the Bleany and Bowers equation[34] (shown below) for dinuclear formulation ($2J = -555$ cm^{-1}, $g = 2.14$, $N\alpha = 60 \times 10^6$ cgsu).

$$\chi = \frac{Ng^2\beta^2}{3kT}\left(1 + \frac{1}{3}e^{2J/kT}\right)^{-1} + N\alpha$$

χ = susceptibility per g atom of copper

J = exchange integral. This is equal to one-half of the singlet-triplet splitting. If J is negative, the compound shows antiferromagnetic behavior.

g = spectroscopic splitting factor or Landé splitting factor

$N\alpha$ = temperature independent paramagnetism

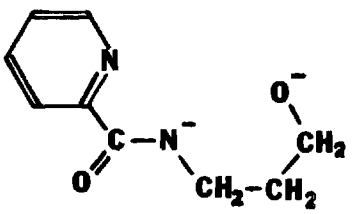
β = Bohr magneton

N = Avogadro's number

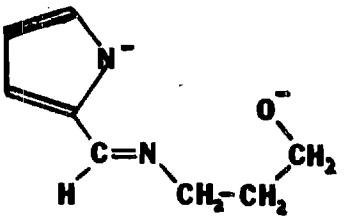
k = Boltzmann's constant

T = absolute temperature

The geometry of the ligand, PIPA, is very similar to that of the Schiff base, PYPA, obtained by condensation of pyrrole-2-carboxaldehyde and 3-amino-1-propanol (Figure 10); and the copper complexes of both ligands show similar magnetic behavior. Thus, it is probable that the structures of the two complexes are similar and that $[CuPIPA]_2$ also contains planar, four coordinate copper ions bridged by the alkoxide groups into a planar, four-membered Cu_2O_2 ring.[35]



PIPA



PYPA

Figure 10. The Dianion of N-(Picolinoyl)-3-amino-1-propanol, PIPA, and the Dianion of the Imine Formed by Pyrrole-2-carboxaldehyde and 3-Amino-1-propanol, PYPA

A blue hydrated compound, $CuPIPA \cdot 2H_2O$, was isolated and, although its magnetic susceptibility was considerably higher than that of CuPIPA at all temperatures, the hydrate also exhibited antiferromagnetic behavior; however, attempts to describe the temperature variation of the magnetic susceptibility of the hydrate in terms of the binuclear formulation were unsuccessful. The best agreement with the experimental values was obtained with a tetrameric ring formulation ($2J = -128$ cm^{-1}, $g = 2.08$), but even that formulation did not agree perfectly over the temperature range studied and the possibility of two or more kinds of magnetic interactions was suggested.

Because of the weaker magnetic coupling and lack of agreement of the magnetic properties with any assumed structure, a crystal structure analysis of the hydrated complex was undertaken.

This work is a systematic structural and magnetic study of several different types of polynuclear metal complexes with aminoalcohols and iminoalcohols as ligands. The work will be described in the four categories shown below.

1) Hydrogen-bonded dinuclear complexes in compounds of the general formula $MM'(Eta)_n(EtaH)_{6-n}X_2$.

2) Hydrogen-bonded dinuclear complexes in compounds of the general formula $Cu(L)(LH)X \cdot nH_2O$; where L represents the anion of 2-aminoethanol or a substituted 2-aminoethanol, $X = NO_3^-$ or ClO_4^-, and $n = 0$ or 1.

3) A tetrameric cobalt complex with 2,2′-dihydroxydiethylamine.

4) The hydrated copper(II) complex of the imine ligand, PIPA.

CHAPTER II

EXPERIMENTS AND RESULTS

Analytical Procedures

Elemental Analysis for C, H, and N

All elemental analyses for C, H, and N were performed by Atlantic Microlab, Inc. in Atlanta, Georgia.

Analysis for Cobalt(II)

The determination of cobalt(II) was carried out by a potentiometric method[36] in which a platinum electrode and a calomel electrode were used. A 0.1 to 0.2 g sample of substance was dissolved in a solution containing 10 ml of concentrated NH_3 and 1 g of NH_4Cl, and a measured amount of a standardized solution of $K_3[Fe(CN)_6]$ was added. The solution was then titrated with a standardized solution of $CoCl_2$. This procedure was carried out in a stream of nitrogen in order to exclude oxygen.

Total Cobalt Analysis

Elemental analyses for total cobalt were performed by the Analytical Chemistry research group of Georgia Tech, using atomic absorption spectroscopy. Total cobalt analysis was also carried out by a potentiometric titration in which the cobalt was first reduced to the divalent state by heating with an excess of concentrated hydrochloric acid. This Co(II) solution was then neutralized and titrated by the procedure described previously.

Analysis for Nickel

Nickel, in the form of bis(dimethylglyoximato) nickel(II), was analyzed by a spectrophotometric method.

Preparation of Compounds

$MM'(Eta)_n(EtaH)_{6-n}(ClO_4)_2$ Compounds

For M = M′ = Ni: The compound was prepared by a slight modification of Kida's method.[11] Solutions of 2.0 g (5.46 mmole) of $Ni(ClO_4)_2 \cdot 6H_2O$ in 30 ml ethanol and 3.2 g (52.4 mmole) of 2-aminoethanol in 20 ml ethanol were warmed to about 60°C and mixed. The resulting solution was filtered while hot and set aside to cool slowly in a Dewar flask; it yielded well-formed blue octahedral crystals. Anal. Calc'd for $NiC_6H_{20}N_3O_7Cl$: C, 21.17; H, 5.92; N, 12.34. Found: C, 21.24; H, 5.97; N, 12.31.

For M = Ni and M′ = Fe, Mn, Zn, and Co, M = Co and M′ = Fe, Mn, Mg, Zn, and Ni: Methanol solutions of 10 mmole of $M(ClO_4)_2 \cdot 6H_2O$ and 95 mmole of 2-aminoethanol were warmed and mixed. A methanol solution of 5 mmole of $M'(ClO_4)_m \cdot nH_2O$ or $M'(OAc)_2 \cdot nH_2O$ was rapidly added to the solution of $M(ClO_4)_2 \cdot 6H_2O$ and 2-aminoethanol. The resulting solution was filtered while hot and set aside to cool. Analytical data are presented in Table 3.

For M = Ni and M′ = Cr: To the methanol solution of 5 mmole of $Ni(ClO_4)_2 \cdot 6H_2O$, 10 mmole of powdered $Cr(Eta)_3 \cdot 3H_2O$ was added. The solution was heated at about 60°C for 15 minutes with continuous stirring. The solution was filtered and then set aside to cool. Analytical results are in Table 3.

Table 3. Analytical Results of $MM'(Eta)_n(EtaH)_{6-n}(ClO_4)_2$[a]

M	M′	Color	C(%)		H(%)		N(%)		Ni(%)		Co(II)(%)		Total Co(%)	
			obs	calc'd	obs	calc'd	obs	calc'd	obs	calc'd	obs	calc'd	obs	calc'd
Ni	Cr	violet	21.10	21.41	5.82	5.84	11.91	12.48	6.40	8.72	--	--	--	--
Ni	Fe	gray	20.94	21.29	5.75	5.81	11.82	12.42	9.83	8.67	--	--	--	--
Ni	Mn	brown	20.81	21.35	5.83	5.97	12.20	12.45	10.18	8.70	--	--	--	--
Ni	Zn	violet	21.01	21.03	5.91	5.88	12.30	12.26	12.45	8.57	--	--	--	--
Ni	Co	violet		21.24		5.94		12.38	9.17	8.65		8.68		8.68
Co	Co[b]	pink	21.38	21.22	6.08	5.94	12.25	12.37	--	--	16.64	17.35	16.94	17.35
Co	Co	violet	21.24	21.22	6.00	5.94	12.42	12.37	--	--	5.17	17.35	17.30	17.35
Co	Fe	violet	20.79	21.28	5.82	5.81	12.06	12.41	--	--		8.70	13.55	8.70
Co	Mn	violet	20.84	21.35	5.76	5.97	12.11	12.45	--	--		8.73	15.65	8.73
Co	Mg	violet	21.15	22.36	5.91	6.26	12.20	13.04	--	--	8.27	9.14	16.67	9.14
Co	Zn	violet	20.96	21.02	5.87	5.88	12.10	12.26	--	--	3.81	8.59	8.59	8.59
Co	Ni	violet		21.24		5.94		12.38	7.02	8.65		8.68		8.68

[a] All analytical values were calculated assuming Ni(II), Co(II), Cr(III), Fe(III), Mn(II), Zn(II), and Mg(II).

[b] This compound was prepared under a nitrogen atmosphere. All other cobalt compounds were prepared under ordinary atmosphere.

For M = M′ = Co(II): The preparation of this compound by the published method[11] was attempted, but the product was always a mixture of cobalt(II) and cobalt(III) as shown in Table 3. Only when all procedures were carried out in a stream of nitrogen was $Co(II)(Eta)(EtaH)_2ClO_4$ obtained. Analytical results are presented in Table 3. When all procedures were carried out in a stream of oxygen, $Co(III)_2(Eta)_3(EtaH)_3(ClO_4)_3$ was obtained. Anal. Calc'd for $Co_2C_{12}H_{39}N_6O_6(ClO_4)_3$: C, 18.46; H, 5.05; N, 10.78. Found: C, 18.39; H, 4.96; N, 10.65.

$Cu(Eta)(EtaH)NO_3$

This compound was prepared by a slight modification of the published method.[11] To 2.0 g (8.3 mmole) of $Cu(NO_3)_2 \cdot 3H_2O$ in 10 ml of dry methanol was added 2.7 g (44.2 mmole) of 2-aminoethanol in 16 ml of dry methanol. The mixture was heated, filtered, and set aside to cool. After one week, the large blue prismatic crystals which formed were filtered and washed with absolute ethanol. Anal. Calc'd for $CuC_4H_{13}N_3O_5$: C, 19.47; H, 5.31; N, 17.03. Found: C, 19.44; H, 5.31; N, 17.09.

$Cu(\ell\text{-Eph})_2 \cdot 2/3\ C_6H_6$

The compound was prepared by the published method.[21] To a solution of 5.0 g (20 mmole) of $CuSO_4 \cdot 5H_2O$ and 4.0 g (26.1 mmole) of ℓ-ephedrine in 100 ml of water was added 20 ml of 20% aqueous NaOH. The resulting blue slurry was extracted with benzene to give a violet solution. This benzene solution was then dried with Na_2SO_4. Repeated evaporation and crystallization of benzene solutions removed traces of water and hexagonal platelets were obtained. For identification, the space group and cell parameters were determined and were found to be identical to the

reported values.

$Cu(\ell\text{-Eph})(\ell\text{-EphH})ClO_4 \cdot H_2O$

To 3.66 g (10 mmole) of $Cu(ClO_4)_2 \cdot 6H_2O$ in 30 ml of dry methanol was added 6.46 g (40 mmole) of ℓ-ephedrine in 40 ml of dry methanol. The mixture was heated, filtered, and set aside to cool. After several days, the large triangular prismatic crystals that formed were filtered. Anal. Calc'd for $[CuC_{20}H_{29}N_2O_2]ClO_4 \cdot H_2O$: C, 47.06; H, 6.12; N, 5.49. Found: C, 47.86; H, 5.83; N, 5.44.

$Cu(Mep)(MepH)NO_3 \cdot H_2O$

To a solution of 4.0 g (16.6 mmole) of $Cu(NO_3)_2 \cdot 3H_2O$ in 50 ml of a mixed solvent (acetone: ethanol = 2:1) was added 8.0 g (89.9 mmole) of 2-amino-2-methyl-1-propanol (abbreviated MepH). The resulting solution was filtered to remove thin violet plates and kept for two days. The blue prismatic crystals which formed were filtered by suction and washed with ethanol. Anal. Calc'd for $CuC_8H_{23}N_3O_6$: C, 29.94; H, 7.23; N, 13.10. Found: C, 30.16; H, 7.20; N, 13.15.

$Cu(Dme)(DmeH)ClO_4$

To a solution of 4.0 g (10.9 mmole) of $Cu(ClO_4)_2 \cdot 6H_2O$ in 60 ml of dry methanol was added 8.0 g (89.9 mmole) of N,N′-dimethyl-2-aminoethanol (abbreviated DmeH). The resulting solution was heated with continuous stirring and filtered. Dark blue needle-shaped crystals were obtained. Anal. Calc'd for $[CuC_8H_{21}N_2O_2]ClO_4$: C, 28.24; H, 6.22; N, 8.23. Found: C, 28.46; H, 6.30; N, 8.27.

$[Co_2(Deta)_2(DetaH_2)]ClO_4$

This compound was prepared by a slight modification of the

published method.[25] A solution of 3.66 g (10 mmole) of $Co(ClO_4)_2 \cdot 6H_2O$ in 15 ml water was mixed with a solution of 6.30 g (60 mmole) of 2,2′-dihydroxydiethylamine in 30 ml of methanol. The resulting pink solution was air-oxidized and filtered. After one week, dark green needle-shaped crystals were obtained. Anal. Calc'd for $Co_2C_{12}H_{31}N_3O_{11}Cl$: C, 27.26; H, 5.53; N, 7.95. Found: C, 26.51; H, 5.76; N, 7.74.

$CuPIPA \cdot 2H_2O$

The method of Ojima[32] was used to synthesize $CuPIPA \cdot 2H_2O$. Large blue diamond-shaped platelets, adequate for X-ray structural analysis, were obtained by recrystallization from water. The crystals gradually change to dark green on heating above 150°C and melt at 260-262°C. Anal. Calc'd for $CuC_9H_{14}N_2O_4$: C, 38.92; H, 5.08; N, 10.09. Found: C, 38.73; H, 5.17; N, 10.19.

Magnetic Studies

The magnetic susceptibilities of compounds were determined by the Faraday method using $HgCo(NCS)_4$ as calibrant. Diamagnetic corrections were applied using tabulated values.[37]

Table 4 lists compounds prepared in this study with name, diamagnetic correction (χ_{dia}) of the sample, and effective magnetic moment per g atom of metal (μ_{eff}) calculated at 296, 195, and 93°K. Tables 5 and 6 list magnetic susceptibilities (χ_m^{corr}) and effective magnetic moments per g atom of metal at various temperatures from 298 to 93°K for NiNiEtaP, CoDeta, CuDme, CuEta, CuMep, and Cu(ℓ-Eph). These abbreviations are listed in Table 2.

Table 4. Diamagnetic Corrections (χ_{dia}) and Effective Magnetic Moment (μ_{eff}) at 298, 195, and 93 °K, for Complexes Prepared

	Xdia X 10^6cgs	μeff BM 298°K	195°K	93°K
$Ni(Eta)(EtaH)_2Cl O_4$	167.0	3.16	3.13	3.04
$NiCr(Eta)_n(EtaH)_{6-n}(Cl O_4)_2$	327.4	5.36	5.28	5.11
$Co(Eta)(EtaH)_2Cl O_4$	167.0	4.69	4.71	4.21
$Co(Eta)_n(EtaH)_{3-n}Cl O_4$ [a]	167.0	2.91	2.88	2.70
$Cu(Eta)(EtaH)NO_3$	114.2	1.78	1.74	1.59
$Cu(\ell\text{-}Eph)_2 \cdot 2/3\ C_6H_6$	171.1	1.75	1.76	1.75
$Cu(\ell\text{-}Eph)(\ell\text{-}EphH)Cl O_4 \cdot H_2O$	283.1	1.93	1.87	1.73
$Cu(Mep)(MepH)NO_3 \cdot H_2O$	161.6	1.85	1.77	1.57
$Cu(Dme)(DmeH)Cl O_4$	174.7	2.02	1.88	1.31
$Co_2(Deta)_2(DetaH_2)Cl O_4$ [b]	258.9	5.19	5.19	5.07
$CuPIPA \cdot 2H_2O$	157.0	1.48	1.38	0.70

[a] This compound was prepared by Kida's method.

[b] Effective magnetic moments per gram atom of Co(II) were calculated assuming Co(III) was diamagnetic.

Table 5. Corrected Molar Magnetic Susceptibilities (X_m^{corr}) and Effective Magnetic Moments (μeff) at Various Temperatures for the Formula Units of: $Ni(Eta)(EtaH)_2Cl0_4$, $Co_2(Deta)_2(DetaH_2)Cl0_4$[a], and $Cu(Dme)(DmeH)Cl0_4$

$Ni(Eta)(EtaH)_2Cl0_4$			$Co_2(Deta)_2(DetaH_2)Cl0_4$			$Cu(Dme)(DmeH)Cl0_4$		
T°K	$X_m^{corr} \times 10^3$ cgs	μeff	T°K	$X_m^{corr} \times 10^3$ cgs	μeff	T°K	$X_m^{corr} \times 10^3$ cgs	μeff
298	4.177	3.16	298	11.18	5.19	298	1.705	2.02
283	4.365	3.16	253	13.16	5.18	293	1.713	2.02
243	5.040	3.15	213	15.74	5.20	283	1.762	2.01
223	5.506	3.14	183	18.18	5.18	273	1.805	2.00
203	6.008	3.14	163	20.45	5.19	263	1.867	1.99
183	6.624	3.12	143	23.19	5.17	253	1.932	1.99
153	7.932	3.12	133	24.67	5.15	243	1.988	1.97
143	8.392	3.11	123	26.38	5.12	233	2.047	1.96
133	8.898	3.09	113	28.49	5.10	223	2.088	1.94
113	10.40	3.08	103	31.20	5.09	213	2.156	1.93
104	11.40	3.09	97	33.60	5.09	203	2.204	1.90
93	12.33	3.04	95	33.52	5.07	193	2.276	1.88
						183	2.334	1.86
						173	2.401	1.83
						163	2.457	1.80
						153	2.497	1.76
						138	2.500	1.67
						133	2.500	1.64
						123	2.464	1.56
						113	2.428	1.49
						103	2.386	1.41
						93	2.283	1.31

[a]Effective magnetic moments per gram atom of Co(II) were calculated assuming Co(III) was diamagnetic.

Table 6. Corrected Molar Magnetic Susceptibilities (X_m^{corr}) and Effective Magnetic Moments (μeff) at Various Temperatures for the Formula Units of: $Cu(Eta)(EtaH)NO_3$, $Cu(Mep)(MepH)NO_3 \cdot H_2O$, and $Cu(\ell\text{-Eph})(\ell\text{-EphH})C\ell O_4 \cdot H_2O$

$Cu(Eta)(EtaH)NO_3$			$Cu(Mep)(MepH)NO_3 \cdot H_2O$			$Cu(\ell\text{-Eph})(\ell\text{-EphH})C\ell O_4 \cdot H_2O$		
T°K	$X_m^{corr} \times 10^3$ cgs	μeff	T°K	$X_m^{corr} \times 10^3$ cgs	μeff	T°K	$X_m^{corr} \times 10^3$ cgs	μeff
298	1.314	1.78	298	1.415	1.85	299	1.543	1.93
293	1.355	1.79	293	1.432	1.84	295	1.553	1.92
283	1.406	1.79	283	1.464	1.83	283	1.599	1.91
273	1.442	1.78	273	1.525	1.83	273	1.649	1.91
263	1.484	1.78	263	1.565	1.82	263	1.705	1.90
253	1.534	1.77	253	1.629	1.82	253	1.767	1.90
243	1.592	1.75	243	1.675	1.81	243	1.809	1.88
233	1.665	1.75	233	1.719	1.80	233	1.906	1.89
223	1.729	1.74	223	1.782	1.79	223	1.974	1.88
213	1.775	1.75	213	1.855	1.79	213	2.058	1.88
203	1.875	1.75	203	1.936	1.73	203	2.147	1.88
193	1.938	1.74	193	2.019	1.77	193	2.246	1.87
183	2.060	1.74	183	2.111	1.77	183	2.353	1.86
173	2.131	1.73	173	2.192	1.75	173	2.466	1.86
163	2.233	1.71	163	2.326	1.75	163	2.595	1.85
153	2.368	1.71	153	2.422	1.73	153	2.723	1.83
143	2.484	1.69	143	2.545	1.71	143	2.883	1.82
133	2.625	1.68	133	2.658	1.69	133	3.115	1.83
123	2.774	1.66	123	2.785	1.66	123	3.297	1.81
113	2.996	1.65	113	2.930	1.63	113	3.462	1.78
103	3.117	1.61	103	3.145	1.62	103	3.739	1.76
93	3.373	1.59	93	3.265	1.57	93	4.005	1.73
91	3.424	1.59						

Absorption Spectra

Absorption spectra in the visible region for CuEta, CuMep, Cu(ℓ-Eph), and CuDme were measured by the opal glass method[38] using a Cary 14 spectrophotometer. Instead of opal glass, filter paper was used. Finely powdered samples were smeared and placed just in front of the photomultiplier housing of the Cary 14. Plain filter paper without sample was used as reference. Absorption spectra of these compounds are shown in Figure 11.

Crystallographic Studies

General

A crystal with the approximate dimensions shown in Table 7 was mounted on a glass fiber using epoxy cement or nail polish, usually such that the longest dimension was approximately parallel to the fiber axis.

For NiNiEtaP and CuPIPA·$2H_2O$, precession photographs were taken to determine space groups. Each mounted crystal was then transferred to a Picker automated diffractometer and about 15 reflections were centered manually and used to refine cell parameters by a least-square procedure. In both the cell refinement and the actual data collection, Zr-filtered molybdenum Kα radiation (λ = 0.70926Å) was used. The cell parameters are shown in Table 7. The experimental densities of these complexes were determined by flotation in carbon tetrachloride-ethylene bromide mixtures. The intensities were measured by a scintillation counter mounted 26.5 cm from the crystal and a source-crystal distance of 21.0 cm; the intensities were collected by the θ-2θ scan technique

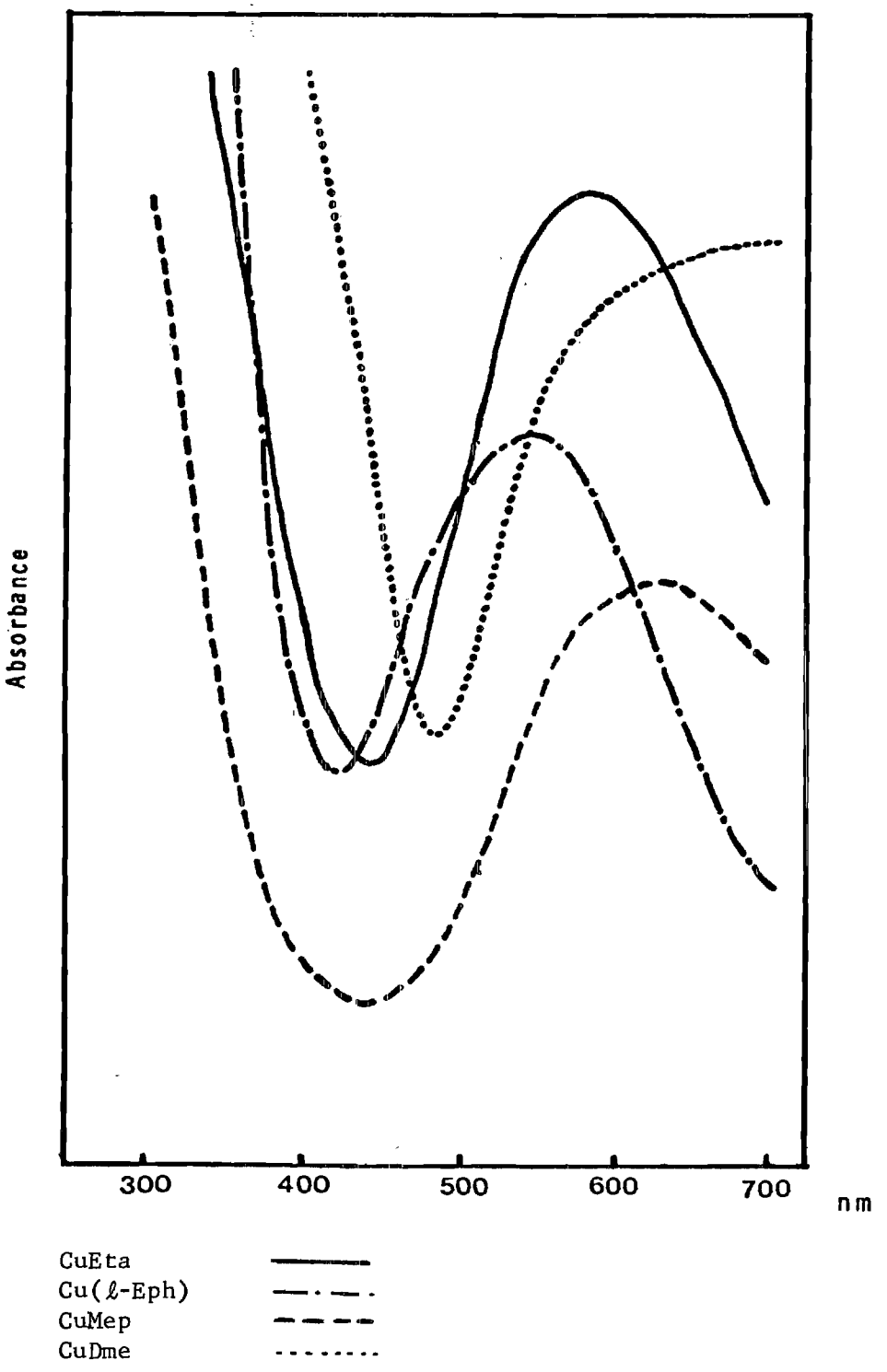


Figure 11. Absorption Spectra of CuEta, CuMep, Cu(ℓ-Eph), and CuDme

Table 7. Crystallographic Data for $Ni(Eta)(EtaH)_2Cl O_4$ and Cu PIPA · $2H_2O$

	$Ni(Eta)(EtaH)_2Cl O_4$	CuPIPA · $2H_2O$
Color	Blue	Blue
Shape	Square pyramidal	Diamond, plate
Size	.50 x .50 x .35	.22 x .10 x .36
Direction mounted	One of the cubic axis	Parallel to h,0,2h
Precession photographs taken	hk0,hkl,h0ℓ,h1ℓ,h2ℓ	h0ℓ,h1ℓ,h2ℓ,hk2h
Systematic absence	0kℓ(k = 2n+1)	hkℓ(h+k = 2n+1)
	h0ℓ(h = 2n+1)	h0ℓ(ℓ = 2n+1)
	hk0(h = 2n)	
Space group	Pa3(No.205)	Cc(No.9) or C2/c(No.15)*
No. of reflections aligned	14	16
Unit cell parameter	a = 13.85(1)	a = 20.328(7)
		b = 7.317(3)
		c = 16.862(3)
		β = 119.58(2)
Calculated density $g \cdot cm^{-3}$	1.67	1.67
Obs. density $g \cdot cm^{-3}$	1.65	1.69
Take-off angle	1.8°	1.6°
Standard reflection	400, 004, 040	040, $\overline{4}$08, 400, 050
Decomposition factor	24%	6%
No. of reflections corrected	ca. 600	ca. 4000
P	0.03	0.02
No. of reflections accepted	371	1369

*Successful refinement of the structure in C2/c verified the assumption of the centrosymmetric space group, C2/c.

with the takeoff angle shown in Table 7 and a scan rate of 1° min^{-1}. For each reflection out to a maximum 2θ angle of 50°, a symmetrical scan of 2.0° was taken about the calculated 2θ position. Stationary background counts of 20 seconds were taken at the beginning (bgd1) and at the end (bgd2) of the scan. Calibrated copper attenuators were used in the collection of data. The threshold point was set so that the counting rate would not exceed 10,000 counts/sec. The pulse height analyzer was set for approximately a 90% window centered on the Mo Kα peak. Several reflections were monitored after every 150 reflections as a check on crystal and instrument stability. An isotropic linear decrease in the intensities of standards was observed during data collection and appropriate corrections were applied. All reflections with $2\theta \leqq 50^{\circ}$ were collected in a full quardrant of reciprocal space for CuPIPA·$2H_2O$ and in a full octant for NiNiEtaP. Corrected intensities (CI) were obtained by subtracting three times the actual measured background from the total integrated peak count (CT).

$$CI = CT - 3(bgd1 + bgd2)$$

The factor of 3 in the calculation arises from the peak scan time being three times as long as the total background counting time. The corrected intensities were assigned standard deviations according to the formula,

$$\sigma(I) = [CT + 0.25(tc/tb)^2(bgd1 + bgd2 + 9.0) + (PI)^2 + 4.5]^{\frac{1}{2}}$$

where tc is the scan time, tb is the counting time of each background (either bgd1 or bgd2), the scalar quantities 4.5 and 9.0 account for truncation of the last counting digit by the Picker scalar, P (the "ignorance factor") was assigned values of 0.03 and 0.02 for NiNiEtaP and $CuPIPA \cdot 2H_2O$ respectively. The total number of reflections shown in the last row of Table 7 are the numbers accepted as statistically above background on the basis that $\sigma(I)/CI$ was less than 0.33. Lorentz and polarization corrections were applied in the usual way.

Unit cell parameters and orientation matrices of CuEta, CuMep, Cu(ℓ-Eph), CuDme, and CoDeta were determined on a Syntex $P2_1$ fourcircle diffractometer equipped with a graphite monochrometor (Bragg 2θ angle = 12.2° using Mo Kα radiation at a takeoff angle of 6.75°. Fifteen reflections whose 2θ values ranged from 5.00 to 25.00° were machine-centered and used in least-squares refinement of the lattice parameters and orientation matrix. Axial photographs were taken to check for mirror symmetry. Intensity data for zero and upper levels were collected at a rapid scan and the intensities examined carefully for systematic absences. The unit cell parameters and space groups obtained are shown in Table 8. The calculated densities of these compounds agree well with the experimental densities measured by the flotation method listed in Table 8. Omega scans of several low 2θ angle reflections gave peak widths at half-height indicating a satisfactory mosaic spread for the crystals. Intensity data for these complexes were collected using θ-2θ scans with X-ray source and monochrometor setting identical to those used for determination of the unit cell parameters. A variable scan rate of from 3.5 to 29.3° min^{-1} was used and a scan width of 2.00 or 2.40° was sufficient to collect all

Table 8. Crystallographic Data for $Cu(Eta)(EtaH)NO_3$, $Cu(Mep)(MepH)NO_3 \cdot H_2O$, $Cu(\ell\text{-Eph})(\ell\text{-EphH})ClO_4 \cdot H_2O$, $Cu(Dme)(DmeH)ClO_4$, and $Co_2(Deta)_2(DetaH_2)ClO_4$

	$Cu(Eta)(EtaH)NO_3$	$Cu(Mep)(MepH)NO_3 \cdot H_2O$	$Cu(\ell\text{-Eph})(\ell\text{-EphH})ClO_4 \cdot H_2O$	$Cu(Dme)(DmeH)ClO_4$	$Co_2(Deta)_2(DetaH_2)ClO_4$
Color	dark blue	blue	purple	blue	dark green
Shape	prismatic	needle	trigonal prismatic	needle	needle
Size	.57x.22x.17	.94x.36x.18	.7x.4x.4	.35x.17x.09	.3x.3x.1
The direction mounted	parallel to b^*	parallel to a^*	parallel to c^*	perpendicular to (110)	parallel to a^*
Unit cell parameters	a = 9.990(2) b = 11.454(1) c = 9.977(2) α = 111.10(1) β = 90.02(1) γ = 119.92(1) V = 901.8(2)	a = 6.232(1) b = 14.036(4) c = 17.097(4) β = 105.79(2) V = 1439.1(6)	a = 13.354(7) c = 24.716(6) V = 3817(3)	a = 8.321(2) b = 17.272(7) c = 13.962(5) β = 101.51(3) V = 1966(1)	a = 8.747(2) b = 17.408(4) c = 13.597(3) β = 111.45(2) V = 1926.8(8)
Calc'd density ($g \cdot cm^{-3}$)	1.816	1.481	1.333	1.699	1.81
(No. of metals per unit cell)	(4)	(4)	(6)	(6)	(8)
Obs. density ($g \cdot cm^{-3}$)	1.823	1.476	1.340	1.653	1.80
(Solvents used)	($CC\ell_4$ & $C_2H_2Br_2$)	($CC\ell_4$ & p-xylene)	($CC\ell_4$ & p-xylene)	($CC\ell_4$ & $C_2H_2Br_2$)	($CC\ell_4$ & $C_2H_2Br_2$)
Widths at half-length	.25°	.26°	.32°	.28°	.25°
Systematic absences	none	h0ℓ(ℓ=2n+1) 0k0(k=2n+1)	hkiℓ(no condition) 000ℓ(ℓ=3n±1)	h0ℓ(h+ℓ=2n+1) 0k0(k=2n+1)	h0ℓ(ℓ=2n+1) 0k0(k=2n+1)
Space group	$P\bar{1}$(No.2)	$P2_1/c$(No.14)	$P3_1$(No.145)	$P2_1/n$	$P2_1/c$(No.14)
Scan rate ($deg \cdot min^{-1}$)	7.34-29.30	7.32-29.30	7.32-29.30	4.88-29.30	3.91-29.30
Scan width (deg)	2.00	2.40	2.00	2.00	2.00
Standard reflections	$030, 2\bar{4}1, 1\bar{2}3$	200,004,060 for 1st data set; 008, 080,800 for 2nd data set	009,500,030	006,200,020	400,080,004
No. of reflections collected	3398(hemisphere)	2775 for 1st set 4513 for 2nd set (quadrant)	9542(quadrant)	3900(quadrant)	3804(quadrant)
2θ maxima collected (deg)	50	50 for 1st set 60 for 2nd set	50	50	50
P	0	0	0	0	0
σ(I)/I	<.50	<.33	<.33	<.33	<.50
No. of reflections accepted	2803	2184 for 1st set 2362 for 2nd set	5047	2107	2719

the peak intensity. Stationary background counts were measured at the beginning (bgd1) and at the end (bgd2) of each scan with a total background to scan time ratio, Tr, of 1. There were no significant fluctuations in the intensities of three standard reflections monitored every 97 reflections except in the case of CuMep. Appropriate corrections were applied for the data set of CuMep where marked decomposition occurred. Intensities were calculated from the total scan count, CT, and background counts by the relationship:

$$I = CT - (bgd1 + bgd2)$$

The intensities were assigned standard deviations according to the formula,

$$\sigma(I) = [CT + (bgd1 + bgd2)]^{\frac{1}{2}}$$

From the total reflections collected out to $2\theta = 50.0^{\circ}$, the numbers of reflections in the last row of Table 8 are the numbers accepted as statistically above background on the basis that I was greater than $2\sigma(I)$ or $3\sigma(I)$. Lorentz and polarization corrections were made in the usual way.

All computations were carried out on a UNIVAC 1108 Exec 8 system or on a CDC Cyber 70/74 computer. Programs employed include Carter's cell parameter and diffractometer setting angle program,[39] Zalkin's FORDAP Fourier summation program,[40] Ibers' NUCLS5 modification of the

Busing-Martin-Levy ORFLS full matrix least square program,[41] the Martin-Busing-Levy ORFFE function and error program,[42] Johnson's ORTEP and ORTEPII plotting programs,[43] Stewart's ABSORB absorption correction program from the X-ray 72 system,[44] and various locally written programs.

In the structure factor calculations, the scattering factors were taken from Cromer and Waber's tabulation[45] for all atoms except hydrogen; Stewart's hydrogen atom scattering factors were used.[46] The scattering factors for copper, cobalt, nickel, and chlorine were corrected for the real and imaginary anomalous dispersion components, using the dispersion factors tabulated by Cromer.[47] The agreement factors are defined in the usual way as:

$$R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$$

and

$$R_w = [\Sigma_w(|F_o| - |F_c|)^2/\Sigma_w(|F_o|)^2]^{\frac{1}{2}}$$

In all least-squares refinements, the quantity minimized was $\Sigma_w(|F_o| - |F_c|)^2$. Throughout this thesis, numbers in parentheses following other numbers indicate estimated standard deviations in the least significant digits.

Solutions, Refinements, and Descriptions of the Structures

NiNiEtaP

Atomic coordinates for the nickel and chlorine atoms were deduced from a three-dimensional Patterson synthesis and refined to give the initial residuals, $R = 0.31$ and $R_w = 0.38$. The remaining atoms were located by means of Fourier syntheses and least-squares refinements. A refinement using a weighting scheme based on counting statistics

($w = I/\sigma^2(I)$) and isotropic temperature factors for all non-hydrogen atoms converged with $R = 0.161$ and $R_w = 0.130$.

Consideration of large thermal parameters for the chelate ring atoms and residual electron density in the vicinity of the chelates in difference Fourier maps led to introduction of a disordered model for the structure. Distinct atomic positions supplemental to those initially chosen were evident for oxygen, nitrogen, and one of the two carbon atoms in the chelate group. Isotropic temperature parameters and positional parameters were henceforth refined for each of these three additional disordered atoms. A single variable was refined to describe the occupancies of the disordered "A" and "B" ligands. The final occupancies for "A" and "B" were 0.690(9) and 0.310(9), respectively. The introduction of individually refined occupancy factors for the disordered atoms did not significantly improve the R-factor. Anisotropic thermal parameters for one nickel atom, one chlorine atom, one carbon atom, and oxygen atoms of perchlorate ion were introduced and further refinement reduced R to 0.088 and R_w to 0.064.

In the final refinements, the methylene and amine hydrogens were included (but not refined) in calculated positions of local C_{2v} symmetry (C-H = N-H = 0.95A; X-Y-H = H-Y-H = 109.5). Hydrogens involved in the polynuclear bridge were not located, despite some attempts to do so. The maximum parameter shifts in the final cycle of refinement was 0.03σ (z coordinate of O1B) and the final residuals are $R = 0.073$ and $R_w = 0.052$. The magnitude of the highest feature on a final difference Fourier map, $0.66e\text{Å}^{-3}$, may be compared to the value of $2.6e\text{Å}^{-3}$ for a typical carbon

Table 9. Individual Atomic and Thermal Parameters* for $[Ni(Eta)(EtaH)_2]_2(ClO_4)_2$

Atom	x	y	z	β_{11} or B[Å^2]	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ni	.0955(1)	.0955(1)	.0955(1)	.0047(1)	.0047(1)	.0047(1)	-.0007(1)	-.0007(1)	-.0007(1)
Cl	.2821(2)	.2821(2)	.2821(2)	.0057(1)	.0057(1)	.0057(1)	-.0006(2)	-.0006(2)	-.0006(2)
02	.3392(7)	.3392(7)	.3392(7)	.0120(6)	.0120(6)	.0120(6)	-.0025(7)	-.0025(7)	-.0025(7)
03	.3348(7)	.2127(8)	.2348(9)	.0100(8)	.0146(9)	.0155(11)	.0044(7)	-.0003(7)	-.0056(9)
01A	.136(1)	-.035(1)	.034(1)	6.9(4)					
01B	.141(2)	.012(2)	-.023(2)	6.9(4)					
NA	.234(1)	.133(1)	.051(1)	3.9(3)					
NB	.229(2)	.050(2)	.143(2)	3.9(3)					
ClA	.222(2)	-.031(1)	-.002(2)	5.1(4)					
ClB	.236(4)	-.006(3)	-.030(3)	5.1(4)					
C2	.287(1)	.043(1)	-.044(1)	.006(1)	.013(1)	.008(1)	.001(1)	-.001(1)	-.001(1)

*The form of the anisotropic thermal ellipsoid is: $\exp[-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}\ell^2 - \beta_{12}hk - \beta_{13}k\ell - \beta_{23}k\ell]$.

Symmetry constraints for the atoms lying at (x,x,x) on the three-fold axis (Ni, Cℓ, and 02) dictate occupancy factors of .333 and the temperature factor relationships $\beta_{11} = \beta_{22} = \beta_{33}$ and $\beta_{12} = \beta_{13} = \beta_{23}$.

The occupancy factor, α, for disordered atoms 01A, ClA, and NA refined to the value .690(9). The corresponding value, 1-α, for atoms 01B, ClB, and NB is .310(9).

Table 10. Interatomic Distances for $[Ni(Eta)(EtaH)_2]_2(ClO_4)_2$

Atoms	Distance (Å)	Atoms	Distance (Å)
Ni-NA	2.08(1)	Ni-NB	2.05(3)
Ni-O1A	2.07(1)	Ni-O1B	2.10(3)
O1A-C1A	1.29(2)	O1B-C1B	1.34(5)
C1A-C2	1.50(2)	C1B-C2	1.42(5)
C2-NA	1.45(2)	C2-NB	1.58(3)
Ni-Ni*[a]	4.582(2)	NA-NB	1.72(3)
Ni-Cℓ	4.476(4)	O1A-O1B	1.02(3)
Cℓ-O2	1.37(2)	O1A-C1B	1.69(4)
Cℓ-O3	1.37(1)	O1B-C1A	1.31(3)
		C1A-C1B	0.56(4)
O1A-O1A''[b]	2.73(2)		
O1B-O1B''	2.68(5)		
O1B-O1A''	2.24(3)		

[a] X and X* are related by the inversion operation.

[b] X and X'' are related by the three-fold inversion operation.

Table 11. Interatomic Angles for $[Ni(Eta)(EtaH)_2]_2(ClO_4)_2$

Atoms	Angle (Degrees)	Atoms	Angle (Degrees)
O1A-Ni-NA	81.2(5)	O1B-Ni-NB	79(1)
O1A-Ni-O1A'[a]	89.1(5)	O1B-Ni-O1B'	88(1)
N1A-Ni-N1A'	96.9(4)	N1B-Ni-N1B'	95(1)
Ni-O1A-C1A	112(1)	Ni-O1B-C1B	117(3)
O1A-C1A-C2	115(2)	O1B-C1B-C2	110(4)
C1A-C2-NA	96(1)	C1B-C2-NB	113(2)
C2-NA-Ni	106(1)	C2-NB-Ni	102(1)
O1A-Ni-O1B	28.3(8)	O2-Cℓ-O3	111.8(5)
NA-Ni-NB	49.1(8)	O3-Cℓ-O3'	107.0(5)
NA-C2-NB	69(1)		
C1A-C2-C1B	22(1)		
C2-C1A-O1B	107(2)		
C2-C1B-O1A	110(4)		

[a] X and X' are related by the three-fold operation.

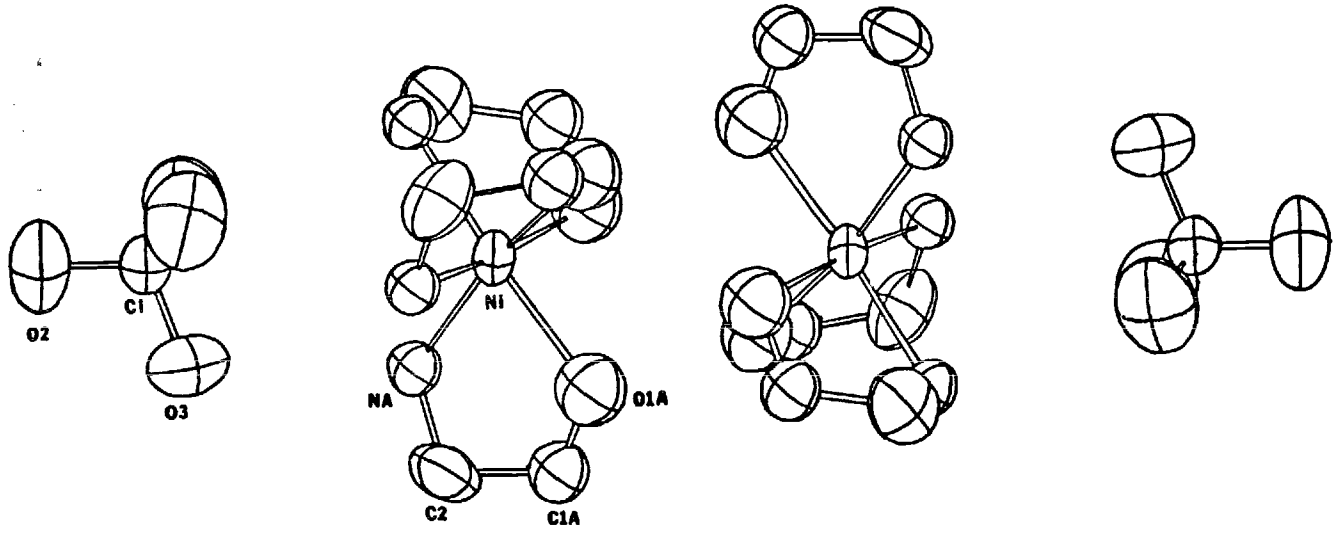


Figure 12. Structure of the Dinuclear Hydrogen-bonded Compound, $[Ni_2(Eta)_2(EtaH)_4](ClO_4)_2$

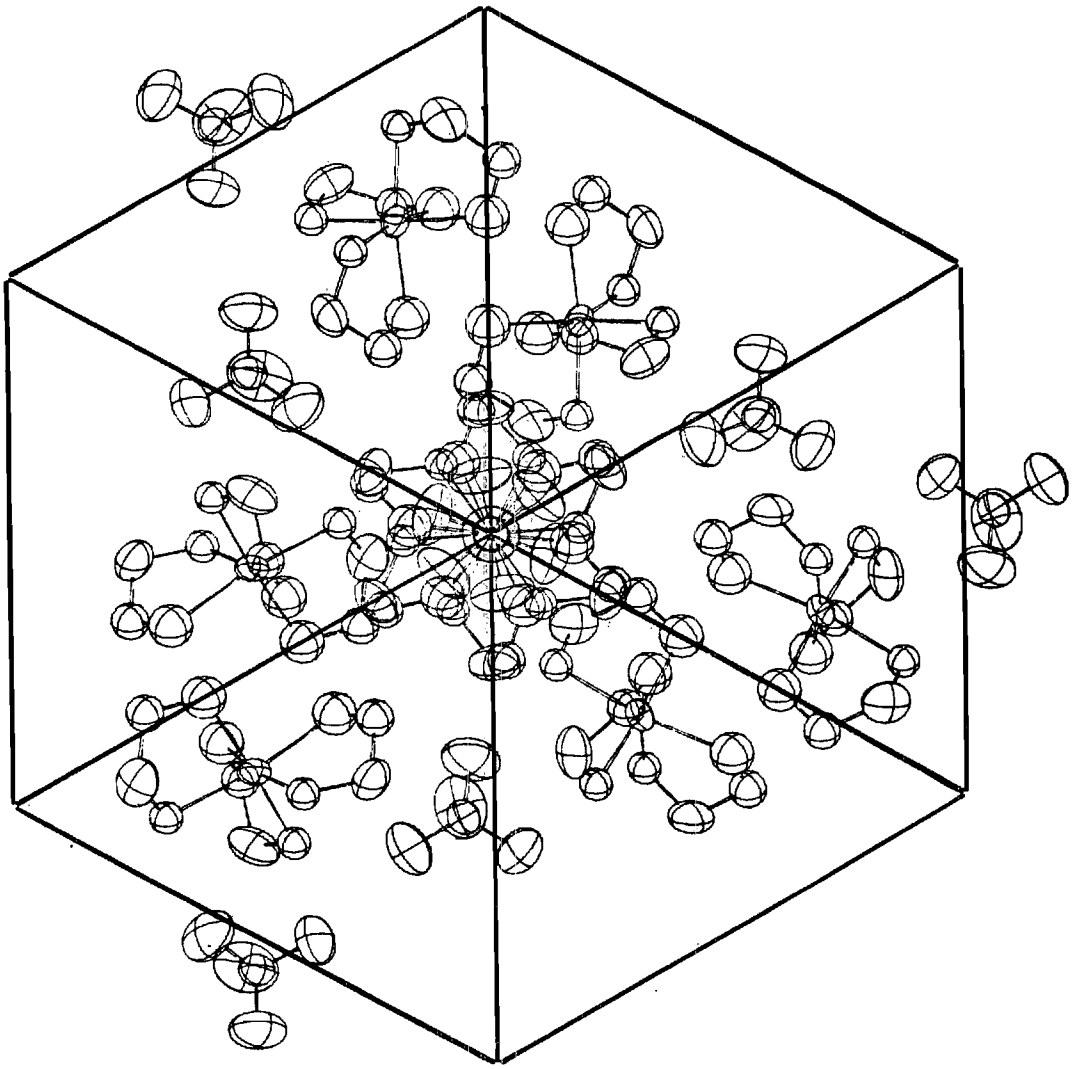


Figure 13. A Perspective View of the Crystal Packing of $[Ni(Eta)(EtaH)_2]_2(ClO_4)_2$

atom in this structure. Final atomic parameters appear in Table 9, selected interatomic bond distances and bond angles are in Tables 10 and 11 respectively. An illustration of the dimeric unit appears in Figure 12. Packing of the ions is shown in Figure 13. Final calculated and observed structure factors appear in the Appendix.

The structural analysis of this compound showed it to be isomorphous with the cobalt-nickel compound.[9] The nickel atoms are located along the three-fold axis of the unit cell on either side of the inversion center. The ClO_4^- anions are along the same axis but they are located farther from the inversion center. The nickel-nickel distance is 4.582(2)Å and the nickel-chlorine distance is 4.476(4)Å.

This structure exhibits a two-fold disorder of the ligand positions, but the occupancy factors refined to value near 1/3 and 2/3 rather than 1/2. These values indicate four ligands of one type and two of another type for each dimeric unit, consistent with the presence of four neutral ligands and only two anion ligands. Consideration of the disorder leads to two short oxygen-oxygen distances indicative of two hydrogen bonds per dimeric unit (O1A-O1A" and O1B-O1B" distances of 2.73(2)Å and 2.68(5)Å are much longer than O1B-O1A" distance of 2.24(3)Å, where X and X" are related by the three-fold inversion operation). O1A-Ni-O1B angle is 28.3(8)° and NA-Ni-NB angle is 49.1(8)°.

CuEta

Two sets of copper atoms and four sets of 2-aminoethanol oxygen and nitrogen atoms were located from a three-dimensional Patterson synthesis. After two cycles of full-matrix least-squares refinement of the coordinates and isotropic temperature factors for these atoms, an R

value of 0.32 and an R_w value of 0.39 were obtained. The remaining non-hydrogen atoms were located from a difference Fourier calculation; carbon atoms and the nitrogen and three oxygen atoms of one set of nitrate ions were in general twofold positions and two nitrate nitrogen atoms were in special positions on inversion centers at (0, 0, 0) and (1/2, 0, 1/2). For these latter nitrates, atom multipliers of 0.5 were assigned to all atoms since the nitrogen atoms occupied special positions and the oxygen atoms were disordered by the inversion symmetry. After several cycles of refinement with anisotropic temperature factors for all atoms except the nitrates in special positions ($R = 0.07$, $R_w = 0.08$), the positions and temperature factors of the atoms of the nitrate at (1/2, 0, 1/2) had refined to unrealistic values. This nitrate ion was introduced as a rigid group and was allowed to refine to a disordered position off of the inversion center; in further refinements of this nitrate with isotropic temperature factors, it was still necessary to fix the temperature factor of one oxygen atom. The oxygen atoms of the nitrate group at (0, 0, 0) were refined with anisotropic temperature factors. Hydrogen atoms were located from a difference Fourier calculation and their positions were refined. With a total of 260 parameters varied, the structure refined to $R = 0.049$ and $R_w = 0.056$. In final cycle of refinement, the maximum parameter shift was 0.33σ (β_{33} of NO22). Residual electron density was located largely in the vicinity of the nitrate groups. Final atomic parameters are listed in Table 12. Final observed and calculated structure factors appear in the Appendix.

The structure of CuEta consists of two independent dinuclear

cations, $[Cu(Eta)(EtaH)]_2^{2+}$, and three independent nitrate ions. Although crystallographically independent, the dinuclear units are virtually identical; Figure 14 is a perspective view of the cation with the atom numbering scheme indicated. Interatomic distances and angles are presented in Tables 13 and 14.

Each copper(II) atom shows square-planar coordination with a cis-arrangement of two 2-aminoethanol chelate ligands. None of the coordinated atoms, Table 15, is more than 0.02Å from the least-squares plane of the copper, oxygen, and nitrogen atoms. The copper-oxygen and copper-nitrogen distances are all in the range of 1.948 to 1.988Å and bond angles at copper range from 84.6 to 99.4°.

The bis-chelated copper(II) complexes, $Cu(Eta)(EtaH)^+$, are associated into hydrogen-bonded dinuclear units about inversion centers at (1/2, 0, 0) and (0, 0, 1/2) with the alcohol groups serving as hydrogen-bond donors and the alkoxide oxygens serving as hydrogen-bond acceptors. The oxygen-oxygen distance of 2.452(6)Å and 2.434(6)Å are shorter than most hydrogen-bonded oxygen-oxygen distances, but are considerably longer than the 2.31Å observed for CuDiimH. The copper-copper distances are 4.940(5)Å and 4.942(5)Å. Cu-O1-O2′ angle and Cu′-O2′-O1 angle are 124.3(2) and 125.1(2)°, respectively. The two coordination planes of the dimers are parallel as a result of the center of inversion (Figure 16). The two parallel coordination planes of the two independent dimers are separated by 1.414 and 1.264Å.

The dimeric units pack together in the solid, Figure 15, with two amine nitrogens of one dimeric unit approaching an alkoxide oxygen and an alcohol oxygen of another dimeric unit. This approach, with nitrogen-

Table 12. Positional and Thermal Parameters for $[Cu(Eta)(EtaH)]_2(NO_3)_2$

Atom	x	y	z	β_{11}[a] or B	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Unit A									
Cu	.3071(1)	-.0077(1)	-.1633(1)	.0083(1)	.0080(1)	.0088(1)	.0043(1)	.0008(1)	.0033(1)
O1	.2971(4)	-.1593(4)	-.1082(4)	.0098(5)	.0077(4)	.0097(5)	.0037(4)	.0002(4)	.0035(4)
C11	.1939(7)	-.3065(6)	-.2218(7)	.0109(8)	.0079(6)	.0120(8)	.0040(6)	-.0001(6)	.0026(6)
C12	.0672(7)	-.3065(6)	-.3027(7)	.0101(8)	.0093(7)	.0112(8)	.0031(6)	-.0010(6)	.0021(6)
N1	.1454(6)	-.1780(5)	-.3418(6)	.0105(6)	.0115(6)	.0096(6)	.0053(5)	.0000(5)	.0031(5)
O2	.4699(4)	.1509(4)	.0145(4)	.0115(5)	.0078(4)	.0097(5)	.0045(4)	.0004(4)	.0030(4)
C21	.5272(7)	.2934(6)	.0149(0)	.0138(9)	.0076(7)	.0144(9)	.0047(6)	-.0016(7)	.0040(6)
C22	.3968(8)	.2881(7)	-.0650(8)	.0148(9)	.0094(7)	.0158(10)	.0067(7)	.0013(8)	.0050(7)
N2	.3240(6)	.1561(5)	-.2056(6)	.0130(7)	.0109(6)	.0118(7)	.0070(6)	.0025(5)	.0054(5)
HC11A[b]	.130 (7)	-.382 (6)	-.181 (7)						
HC11B	.269 (7)	-.324 (6)	-.295 (6)						
HC12A	.001 (7)	-.278 (6)	-.240 (7)						
HC12B	.021 (7)	-.393 (6)	-.396 (7)						
HC21A	.610 (7)	.311 (6)	-.057 (7)						
HC21B	.557 (7)	.371 (6)	.126 (7)						
HC22A	.454 (7)	.384 (6)	-.092 (6)						
HC22B	.320 (7)	.274 (6)	-.029 (7)						
HN1A	.197 (7)	-.194 (7)	-.411 (7)						
HN1B	.071 (7)	-.163 (6)	-.371 (6)						
HN2A	.385 (7)	.162 (6)	-.278 (7)						
HN2B	.222 (7)	.134 (6)	-.244 (7)						
HO2	.601 (7)	.163 (6)	.076 (6)						
Unit B									
Cu	.1563(1)	-.0031(1)	.3083(1)	.0100(1)	.0078(1)	.0076(1)	.0048(1)	.0031(1)	.0034(1)
O1	.1318(4)	.1547(4)	.4459(4)	.0106(5)	.0072(4)	.0100(5)	.0050(4)	.0036(4)	.0036(4)

Table 12. (Continued)

Atom	x	y	z	β_{11}[a] or B	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C11	.2695(7)	.2985(6)	.4822(7)	.0124(8)	.0078(6)	.0118(8)	.0041(6)	.0028(6)	.0043(6)
C12	.3436(8)	.2920(7)	.3497(8)	.0121(8)	.0080(7)	.0132(9)	.0027(6)	.0037(7)	.0052(6)
N1	.3580(6)	.1628(6)	.3015(6)	.0120(7)	.0126(7)	.0112(6)	.0068(6)	.0049(5)	.0065(5)
O2	-.0433(4)	-.1541(4)	.3270(4)	.0093(5)	.0078(4)	.0096(5)	.0039(4)	.0027(4)	.0028(4)
C21	-.0741(8)	-.2994(6)	.2464(7)	.0133(8)	.0081(7)	.0124(8)	.0053(6)	.0032(7)	.0033(6)
C22	.0029(8)	-.3023(7)	.1154(7)	.0175(10)	.0092(7)	.0105(8)	.0077(7)	.0026(7)	.0017(7)
N2	.1650(6)	-.1729(6)	.1685(6)	.0149(8)	.0121(7)	.0106(6)	.0088(6)	.0052(6)	.0052(5)
HC11A	.340 (7)	.319 (6)	.557 (7)						
HC11B	.257 (7)	.381 (6)	.512 (7)						
HC12A	.274 (7)	.279 (6)	.281 (7)						
HC12B	.421 (7)	.358 (7)	.372 (7)						
HC21A	-.172 (7)	-.366 (7)	.217 (7)						
HC21B	-.044 (7)	-.324 (6)	.307 (7)						
HC22A	-.007 (7)	-.392 (7)	.064 (7)						
HC22B	-.042 (7)	-.295 (6)	.058 (7)						
HN1A	.430 (7)	.180 (6)	.361 (7)						
HN1B	.390 (7)	.148 (6)	.221 (7)						
HN2A	.216 (7)	-.185 (7)	.205 (7)						
HN2B	.208 (7)	-.149 (6)	.106 (7)						
HO2	-.095 (6)	-.145 (6)	.456 (7)						
NN1	.2965(6)	-.3806(6)	.3387(7)	.0129(8)	.0141(8)	.0162(9)	.0066(6)	.0035(7)	.0084(7)
ON11	.320 (1)	-.362 (1)	.462 (1)	.035 (2)	.035 (2)	.020 (1)	.003 (1)	-.002 (1)	.011 (1)
ON12	.202 (1)	-.365 (1)	.297 (2)	.028 (2)	.041 (2)	.102 (5)	.015 (2)	.001 (2)	.051 (3)
ON13	.367 (2)	-.420 (2)	.263 (2)	.076 (4)	.059 (3)	.052 (3)	.050 (3)	.047 (3)	.033 (3)
NN2	.000	.000	.000	3.0 (1)					
ON21	-.021 (2)	.009 (2)	.125 (2)	.050 (4)	.031 (3)	.023 (2)	.030 (3)	.025 (3)	.019 (2)
ON22	.083 (2)	-.042 (2)	-.040 (3)	.037 (4)	.047 (4)	.043 (5)	.033 (4)	.032 (4)	.032 (4)
ON23	-.047 (5)	.041 (3)	-.058 (2)	.099 (10)	.054 (6)	.022 (3)	.062 (7)	-.007 (4)	.009 (3)
NN3	.515	-.004	.457	9.1 (2)					

Table 12. (Continued)

Atom	x	y	z	β_{11}[a] or B	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
ON31	.620	-.010	.500	8.4[c] (2)					
ON32	.430	.010	.534	9.4[c]					
ON33	.495	-.012	.338	6.9 (2)					

[a]The form of the thermal ellipsoid expression is exp $[-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl]$.

[b]All hydrogen atoms were assigned isotropic thermal parameters of 3.0.

[c]The thermal parameter of ON32 was not refined.

Table 13. Interatomic Distances (Å) for $[Cu(Eta)(EtaH)]_2(NO_3)_2$

Atoms	Dist	Atoms	Dist
Unit A		**Unit B**	
Cu-Cu'	4.940(5)	Cu-Cu'	4.942(5)
O1-O2'	2.452(6)	O1-O2'	2.434(6)
Cu-O1	1.960(4)	Cu-O1	1.966(4)
Cu-N1	1.985(5)	Cu-N1	1.987(5)
Cu-O2	1.955(5)	Cu-O2	1.948(4)
Cu-N2	1.995(5)	Cu-N2	1.988(5)
O1-C11	1.442(7)	O1-C11	1.433(7)
C11-C12	1.501(8)	C11-C12	1.509(9)
C12-N1	1.481(8)	C12-N1	1.463(8)
O2-C21	1.433(7)	C2-C21	1.427(7)
C21-C22	1.490(9)	C21-C22	1.517(9)
C22-N2	1.470(9)	C22-N2	1.464(9)
C11-HC11A	1.02(6)	C11-HC11A	.91(6)
C11-HC11B	1.08(6)	C11-HC11B	.96(6)
C12-HC12A	1.00(6)	C12-HC12A	.89(6)
C12-HC12B	.97(6)	C12-HC12B	.71(6)
C21-HC21A	1.09(6)	C21-HC21A	.85(6)
C21-HC21B	1.06(6)	C21-HC21B	.86(6)
C22-HC22A	1.09(6)	C21-HC22A	.92(6)
C22-HC22B	.81(6)	C21-HC22B	.78(6)
N1-HN1A	.88(6)	N1-HN1A	.83(6)
N1-HN1B	.91(6)	N1-HN1B	.86(6)
N2-HN2A	.94(6)	N2-HN2A	.72(6)
N2-HN2B	.96(6)	N2-HN2B	.81(6)
O2-HO2	1.37(6)	O2-HO2	1.38(6)
NN1-ON11	1.18(1)		
NN1-ON12	1.15(1)		
NN1-ON13	1.16(1)		
NN2-ON21	1.25(1)		
NN2-ON22	1.20(2)		
NN2-ON23	1.18(2)		

Table 14. Interatomic Angles (deg) for $[Cu(Eta)(EtaH)]_2(NO_3)_2$

Atoms	Angle	Atoms	Angle
Unit A		**Unit B**	
O1-Cu-N1	84.9(2)	O1-Cu-N1	84.6(2)
N1-Cu-N2	98.6(2)	N1-Cu-N2	99.4(2)
O1-Cu-O2	91.4(2)	O1-Cu-O2	91.1(2)
N2-Cu-O2	85.0(2)	N2-Cu-O2	84.9(2)
Cu-O1-C11	111.9(3)	Cu-O1-C11	112.0(3)
O1-C11-C12	108.0(5)	O1-C11-C12	107.5(5)
C11-C12-N1	107.9(5)	C11-C12-N1	108.1(5)
C12-N1-Cu	106.2(4)	C12-N1-Cu	106.9(4)
Cu-O2-C21	111.2(3)	Cu-O2-C21	111.9(3)
O2-C21-C22	109.2(5)	O2-C21-C22	109.1(5)
C21-C22-N2	108.0(5)	C21-C22-N2	107.5(5)
C22-N2-Cu	106.7(4)	C22-N2-Cu	107.1(4)
O2-HO2-O1'	172(6)	O2-HO2-O1'	170(6)
O1N1-NN1-O2N1	119(1)		
O2N1-NN1-O3N1	123(1)		
O1N1-NN1-O3N1	117(1)		
O1N2-NN2-O2N2	116(1)		
O2N2-NN2-O3N2	134(1)		
O1N2-NN2-O3N2	105(1)		

Table 15. Least Square Planes Within the Molecule $[Cu(Eta)(EtaH)]_2(NO_3)_2$[a,b]

Atom	Deviation (Å)	Atom	Deviation (Å)
(a) Plane involving four atoms (O1, O2, N1, and N2) coordinated to Cu (Unit A)			
Equation: -0.833x - 0.241y + 0.498z + 3.456 = 0			
O1	.021	N2	.020
O2	-.021	Cu	.001
N1	-.019		
(b) Plane involving four atoms (O1, O2, N1, and N2) coordinated to Cu (Unit B)			
Equation: 0.554x - 0.321y + 0.769z - 3.394 = 0			
O1	-.011	N2	-.011
O2	.011	Cu	.004
N1	.010		
(c) Plane involving five atoms (O1, O2, N1, N2, and Cu) (Unit A)			
Equation: -0.833x - 0.241y + 0.498z + 3.454 = 0			
O1	.021	N2	.019
O2	-.021	Cu	.000
N1	.019	Cu′	-1.414
(d) Plane involving five atoms (O1, O2, N1, N2, and Cu) (Unit B)			
Equation: 0.553x - 0.321y + 0.769z - 3.395 = 0			
O1	-.012	N2	-.011
O2	.011	Cu	.003
N1	.010	Cu′	-1.264

[a]Direction cosines of the planes refer to the orthogonal axis system a, b, c*.

[b]All atoms weighted at unity.

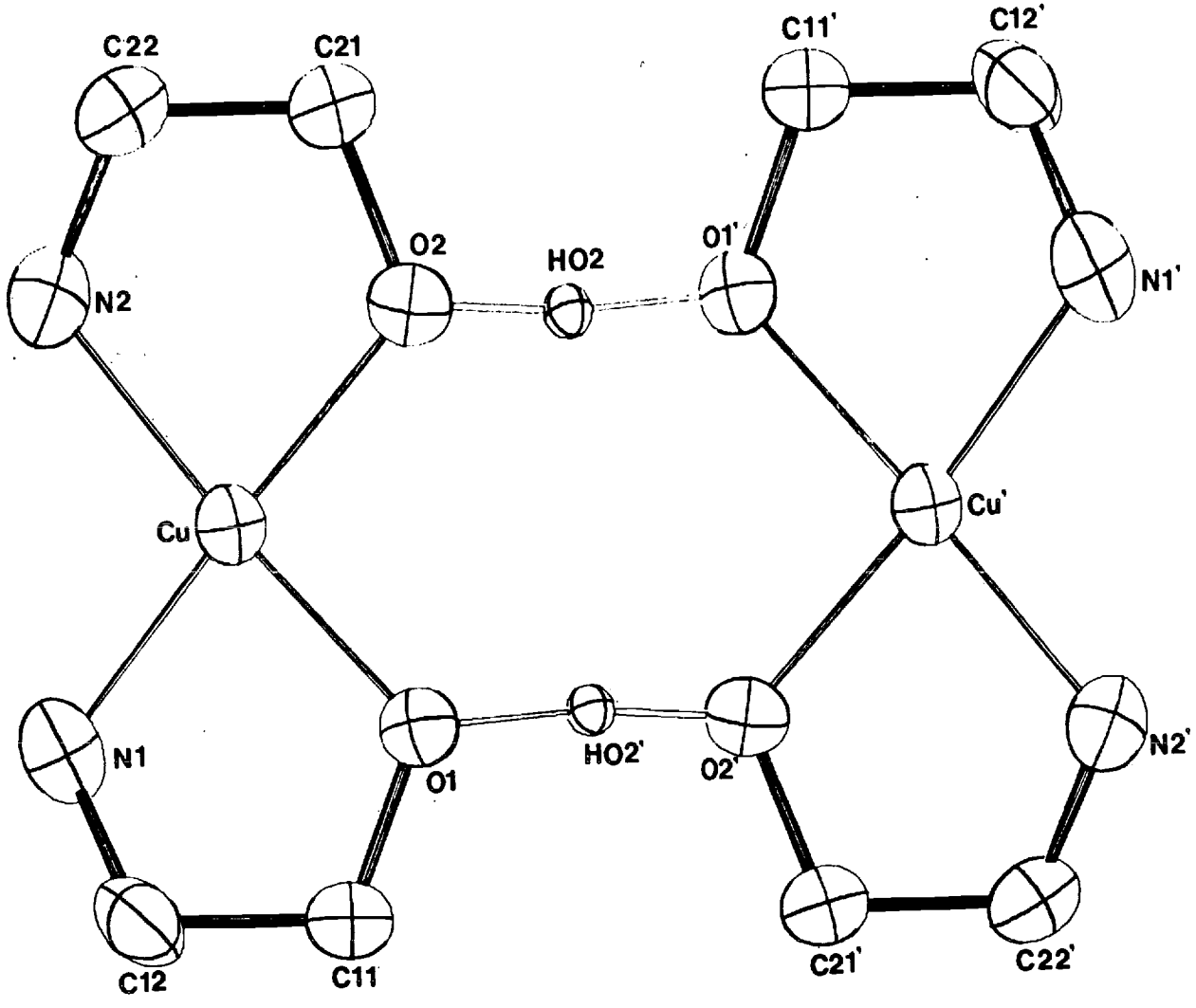


Figure 14. Structure of the Dinuclear Cation, $[Cu(Eta)(EtaH)]_2^{2+}$

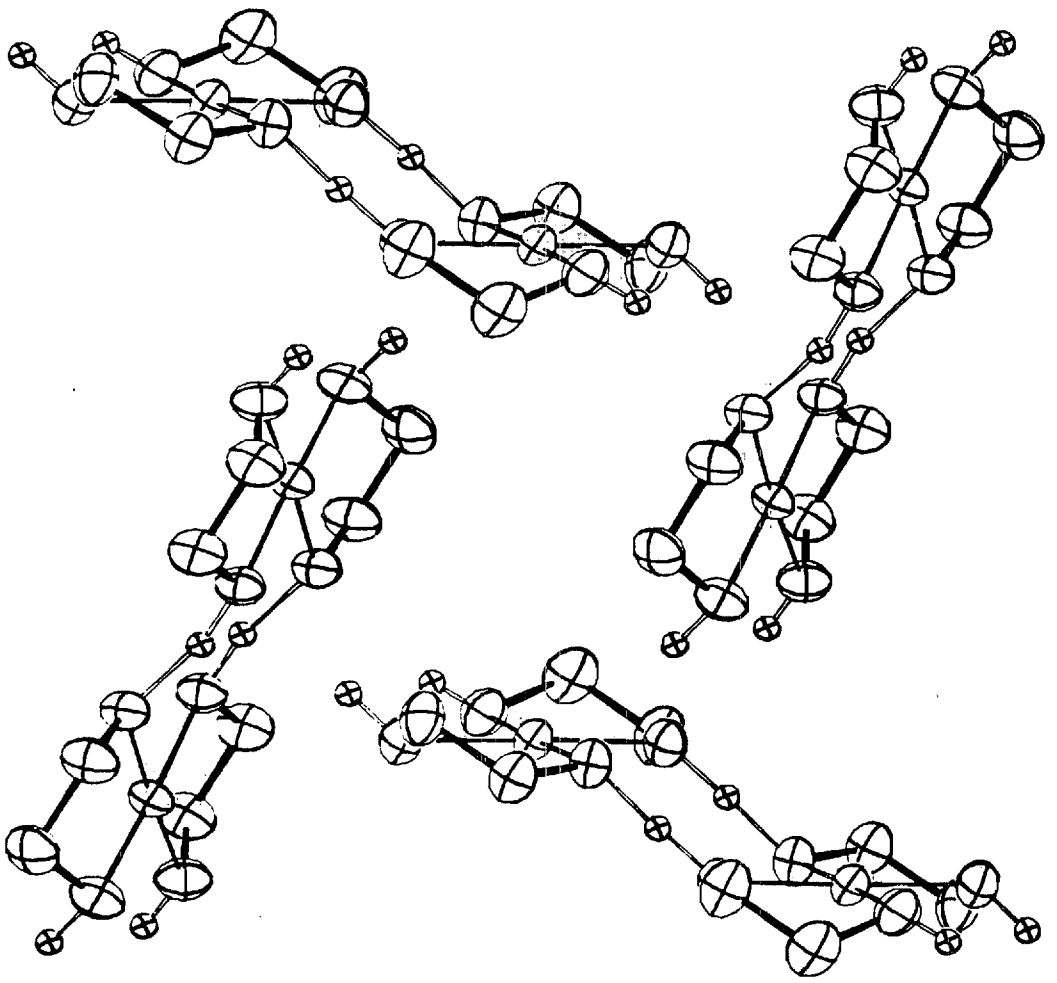


Figure 15. Packing of the Dimeric Cations for CuEta

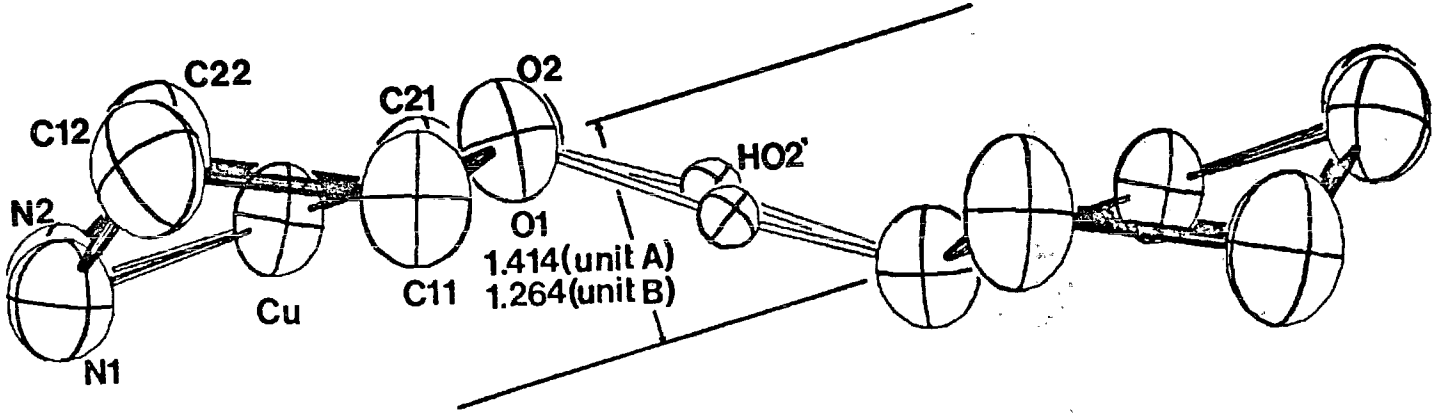


Figure 16. View of the Dinuclear Cation, $[Cu(Eta)(EtaH)]_2^{2+}$, Showing the "Step" Arrangement

oxygen distances ranging from 3.043(7) to 3.124(7)Å, indicates a hydrogen-bonding network in this structure.

CuMep

Atomic coordinates for the copper atom, two sets of oxygen atoms, and two sets of nitrogen atoms were deduced from a three-dimensional Patterson synthesis and refined to give the initial residuals, R = 0.398 and R_w = 0.449. The remaining atoms were located by means of Fourier syntheses and least-squares refinements. A refinement using a weighting scheme and isotropic temperature factors for all non-hydrogen atoms converged with R = 0.138 and R_w = 0.170. Anisotropic thermal parameters were introduced and further refinement reduced R to 0.086 and R_w to 0.110. The eight principal faces of the crystal were identified as the following (distance in millimeters from the center of the crystal to the face is given in parentheses): {011} (0.179), {01$\bar{1}$} (0.090), {001} (0.155), {100} (0.470). Absorption corrections, calculated by the gaussian quadrature method, were applied; corrections on F_2 ranged from 1.20 to 1.44. Refinement with the absorption-corrected data set showed no improvements of R and R_w values. In both data sets (with and without absorption correction) several strong reflections indicated bad agreement between calculated and observed structure factors. A new data set was collected; two crystals were required because of excessive decomposition. Appropriate scaling corrections, based on standard reflections, were applied. Three cycles of full-matrix least-squares refinement, using the coordinates and anisotropic temperature factors of all non-hydrogen atoms of the original data set, reduced R to 0.060 and R_w to 0.055. The 23 hydrogen atoms were located as the principal features on an electron density

map; in subsequent refinements, the hydrogen coordinates were varied but the hydrogen thermal parameters were fixed at 5.0. The positional parameters of two hydrogen atoms bonded to C4 did not refine well and were fixed at calculated positions. The refinement converged to the final values of $R = 0.041$ and $R_w = 0.030$. In the final cycle of refinement, the maximum parameter shift was 0.18σ (z coordinate of H2C1). The major feature on a final difference Fourier map was a peak of $0.32e\text{Å}^{-3}$ about 1.0Å from Cu; this compares to values of approximately $0.40e\text{Å}^{-3}$ for typical hydrogen atoms in this structure. Final atomic parameters are listed in Table 16. Final calculated and observed structure factors appear in the Appendix.

The structure of CuMep is best represented by the formula $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$, and the structure of the cation resembles that of CuEta. Figure 17 is a perspective view of the cation with the atom numbering scheme indicated. Interatomic distances and angles are presented in Tables 17 and 18.

The coordination of the copper is a distorted tetragonal pyramid with a water molecule in the axial position. The position of the copper atom is 0.17Å above the plane, Table 19, formed by the four coordinated atoms of the chelate ligands. The axial copper-oxygen distance (2.313(5)Å) is considerably longer than the copper-oxygen distances in the basal plane (1.932(2) and 1.978(2)Å).

The bis-chelated complexes $Cu(Mep)(MepH)(H_2O)^+$ are associated into hydrogen-bonded dinuclear unit about an inversion center at (-1/2, 0, 0). The oxygen-oxygen distance of 2.516(3)Å is longer than the oxygen-oxygen distances of 2.452(6) and 2.434(6)Å for CuEta. However, the copper-

Table 16. Positional and Thermal Parameters for $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$[a]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	-.21011(6)	-.11258(2)	.07279(2)	.02166(10)	.00260(1)	.00189(1)	-.00042(5)	.00096(2)	-.00008(2)
O1	-.2514(3)	-.0235(1)	.0784(1)	.0251(8)	.0029(1)	.0021(1)	-.0000(2)	.0008(2)	.0000(1)
O2	-.3994(4)	.1227(1)	-.0403(1)	.0257(7)	.0031(7)	.0023(1)	-.0010(2)	.0002(2)	.0000(1)
OW	.1442(5)	.0909(2)	.0576(2)	.0291(9)	.0048(1)	.0037(1)	.0001(3)	.0038(3)	-.0008(1)
N1	-.0923(5)	.1077(2)	.1943(1)	.0276(8)	.0033(1)	.0022(1)	-.0008(3)	.0020(2)	-.0004(1)
N2	-.1963(6)	.2545(2)	.0647(2)	.0236(8)	.0031(1)	.0025(1)	.0000(3)	.0020(2)	-.0003(1)
C1	-.1130(6)	-.0553(2)	.1548(2)	.0278(11)	.0030(1)	.0023(1)	.0008(3)	.0005(3)	.0000(1)
C2	-.1353(5)	.0111(2)	.2226(2)	.0260(10)	.0035(1)	.0019(1)	.0005(3)	.0008(3)	.0003(1)
C3	-.3688(7)	.0109(3)	.2316(2)	.0342(14)	.0050(2)	.0035(1)	-.0004(5)	.0040(4)	.0003(1)
C4	.0355(7)	-.0150(3)	.3021(2)	.0420(15)	.0054(2)	.0025(1)	.0009(5)	-.0010(4)	.0003(1)
C5	-.4753(6)	.2187(2)	-.0591(2)	.0259(10)	.0035(1)	.0027(1)	.0004(3)	.0005(3)	.0005(1)
C6	-.2852(5)	.2867(2)	-.0213(2)	.0231(9)	.0030(1)	.0027(1)	-.0002(3)	.0013(3)	.0003(1)
C7	-.1031(7)	.2797(3)	-.0632(2)	.0315(14)	.0052(2)	.0033(1)	-.0007(5)	.0028(4)	.0006(1)
C8	-.3764(7)	.3881(3)	-.0246(2)	.0385(13)	.0037(1)	.0045(1)	.0013(5)	.0019(4)	.0006(2)
NN	.4208(5)	.2635(2)	.1902(2)	.0292(10)	.0047(1)	.0038(1)	-.0020(3)	.0028(3)	-.0018(1)
ON1	.3529(6)	.2707(2)	.1151(2)	.0514(12)	.0104(2)	.0034(1)	-.0068(4)	.0019(3)	-.0009(1)
ON2	.2893(6)	.2432(3)	.2282(2)	.0532(13)	.0120(3)	.0060(2)	-.0136(5)	.0098(4)	-.0038(2)
ON3	.6201(4)	.2780(2)	.2232(2)	.0262(8)	.0081(2)	.0061(1)	-.0005(3)	.0010(3)	-.0023(1)
HO2	-.514(7)	.088(3)	-.053(2)						
H1W	.212(7)	.133(3)	.066(3)						
H2W	.170(8)	.072(3)	.025(3)						
H1N1	-.140(7)	.152(3)	.222(2)						
H2N1	.042(7)	.120(3)	.203(2)						
H1N2	-.287(7)	.273(3)	.092(2)						
H2N2	-.051(7)	.271(3)	.082(2)						
H1C1	-.151(6)	-.119(3)	.164(2)						
H2C1	.047(7)	-.057(3)	.154(2)						
H1C3	-.388(7)	.052(3)	.268(2)						
H2C3	-.465(7)	.026(3)	.182(3)						
H3C3	-.410(7)	-.047(3)	.245(2)						
H1C4	.017(7)	.024(3)	.341(2)						

Table 16. (Continued)

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
H2C4	.189	-.004	.294						
H3C4	.030	-.007	.317						
H1C5	-.512(6)	.226(3)	-.115(2)						
H2C5	-.608(7)	.232(3)	-.035(2)						
H1C7	-.049(7)	.215(3)	-.064(2)						
H2C7	.024(7)	.320(3)	-.036(2)						
H3C7	-.155(7)	.297(3)	-.118(2)						
H1C8	-.487(7)	.390(3)	.005(2)						
H2C8	.242(7)	.431(3)	-.000(2)						
H3C8	-.447(6)	.406(3)	-.079(2)						

[a]The form of the thermal ellipsoid expression is exp $[-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}\ell^2 - 2\beta_{12}hk - 2\beta_{13}h\ell - 2\beta_{23}k\ell]$. All hydrogen atoms were assigned isotropic thermal parameters of 5.0. The positional parameters of H2C4 and H3C4 were not refined.

Table 17. Interatomic Distances (Å) for $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$[a]

Atoms	Distance	Atoms	Distance
Cu-Cu'	5.156(1)	O2-HO2	.85(4)
Cu-Cu''	4.934(1)	O1''-HO2	1.67(4)
O2-O1''	2.516(3)	N1-H1N1	.89(4)
Cu-O1	1.932(2)	N1-H2N1	.83(4)
Cu-O2	1.978(2)	N2-H1N2	.86(4)
Cu-N1	2.008(3)	N2-H2N2	.90(4)
Cu-N2	2.000(3)	C1-H1C1	.95(4)
Cu-OW	2.313(5)	C1-H2C1	1.00(4)
O1-C1	1.472(3)	C3-H1C3	.86(4)
C1-C2	1.523(4)	C3-H2C3	.91(4)
C2-N1	1.488(4)	C3-H3C3	.90(4)
C2-C3	1.504(5)	C4-H1C1	.89(4)
C2-C4	1.525(4)	C4-H2C2	1.02
O2-C5	1.436(4)	C4-H3C3	.91
C5-C6	1.523(4)	C5-H1C5	.93(4)
C6-N2	1.492(4)	C5-H2C5	1.03(4)
C6-C7	1.502(4)	C7-H1C7	.97(4)
C6-C8	1.528(5)	C7-H2C7	.98(4)
NN-ON1	1.242(4)	C7-H3C7	.94(4)
NN-ON2	1.210(4)	C8-H1C8	.96(5)
NN-ON3	1.234(4)	C8-H2C8	1.02(4)
		C8-H3C8	.94(4)
OW-O2'	3.442(4)		
Cu-ON1	3.733(5)		
Cu-ON2	4.966(6)		
Cu-ON3	3.822(3)		
N1-ON2	2.969(6)		
N2-ON1	3.302(6)		

[a] X and X' are related by the inversion operation. X and X'' are related by inversion, translation operation.

Table 18. Interatomic Angles (degrees) for $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$[a]

Atoms	Degrees	Atoms	Degrees
O1-Cu-N1	86.0(1)	ON1-NN-ON2	119.0(3)
N1-Cu-N2	95.5(1)	ON2-NN-ON3	122.6(3)
O1-Cu-O2	93.9(1)	ON1-NN-ON3	118.5(4)
N2-Cu-O2	83.5(1)	O2-HO2-O1"	177 (4)
OW-Cu-O1	91.1(1)	Cu-O2-O1"	117.2(1)
OW-Cu-O2	103.5(1)	O2-O1"-Cu"	130.6(1)
OW-Cu-N1	91.2(1)		
OW-Cu-N2	93.6(1)		
Cu-O1-C1	107.4(1)		
O1-C1-C2	111.3(2)		
C1-C2-C3	111.6(3)		
C1-C2-C4	110.2(3)		
C2-N1-Cu	108.7(1)		
C3-C2-N1	107.4(3)		
C4-C2-N1	111.4(2)		
Cu-O2-C5	111.0(2)		
O2-C5-C6	108.8(2)		
C5-C6-C7	110.9(3)		
C5-C6-C8	109.3(3)		
C6-N2-Cu	111.1(2)		
C7-C6-N2	108.9(3)		
C8-C6-N2	110.7(3)		

[a] X and X" are related by inversion, translation operation.

Table 19. Least Squares Planes[a,b] for $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$

Atom	Deviation Å	Atom	Deviation Å
(A) The Plane of the Four Atoms Strongly Coordinated to Copper			
Equation $-.970x + .117y + .213Z - 2.208 = 0$			
O1	-.098	N2	-.086
O2	.084	Cu*	-.169
N1	.085		
(B) Basal Plane around Cu			
Equation $-.970x + .118y + .214Z - 2.179 = 0$			
Cu	-.138	N1	.120
O1	-.069	N2	-.051
O2	.113	Cu"*	1.821
(C) Coordination Plane for Dimer			
Equation $-.870x + .325y + .370Z - 2.770 = 0$			
Cu	-.380	Cu"	.264
O1	-.719	O1"	-.225
O2	-.454	O2"	-.307
N1	.191	N1"	.338
N2	.109	N2"	.603
(D) Plane of Nitrate Anion			
Equation $-.224x + .970y + .090Z - 3.485 = 0$			
NN	-.003	ON2	.001
ON1	.001	ON3	.001

[a]Direction cosines of the planes refer to the orthogonal axis system a, b, c*.

[b]Planes are derived using unit weights for all atoms marked without asterisks and zero weights for atoms marked with asterisks.

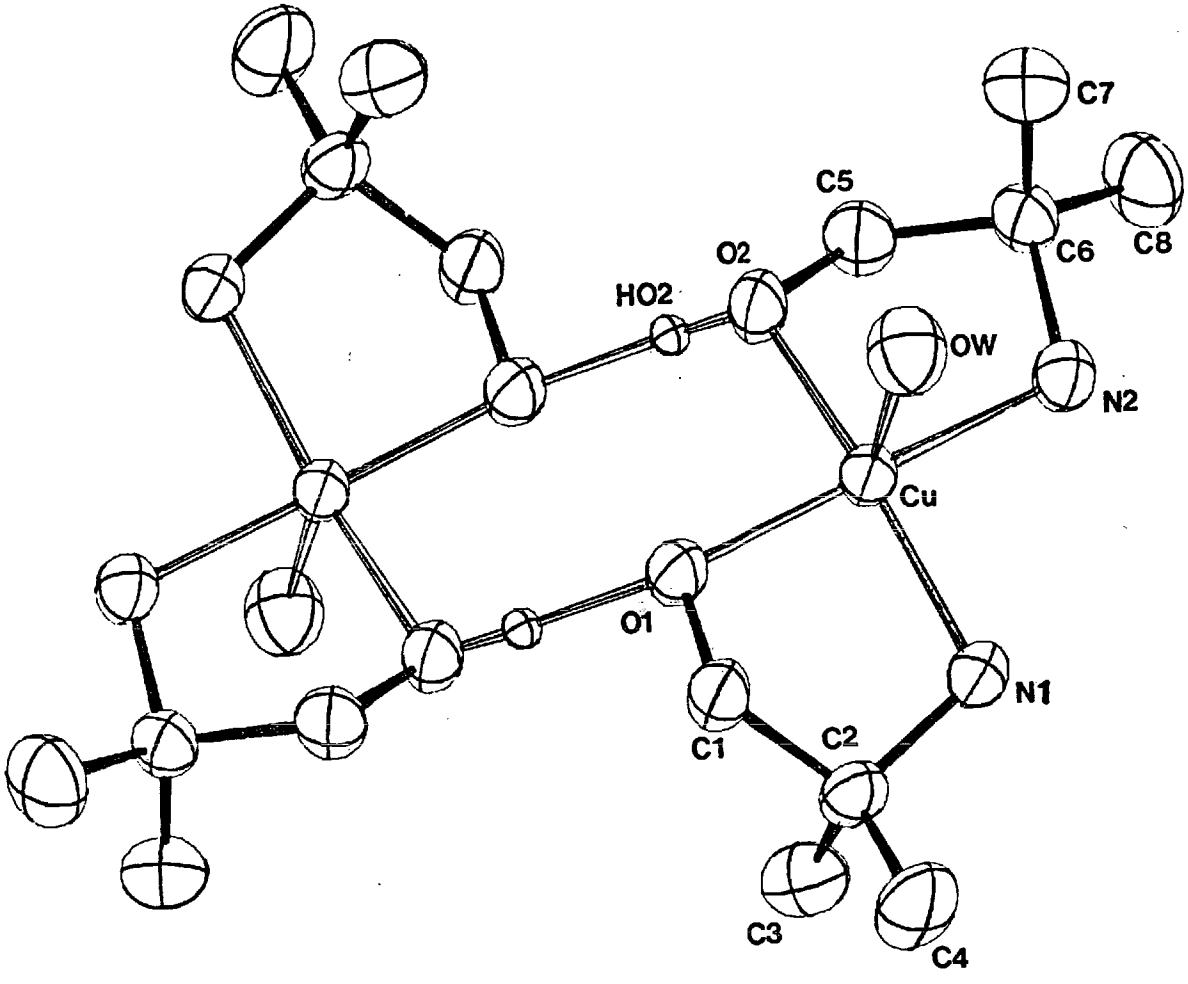


Figure 17. Structure of the Dinuclear Cation, $[Cu(Mep)(MepH)(H_2O)]_2^{2+}$

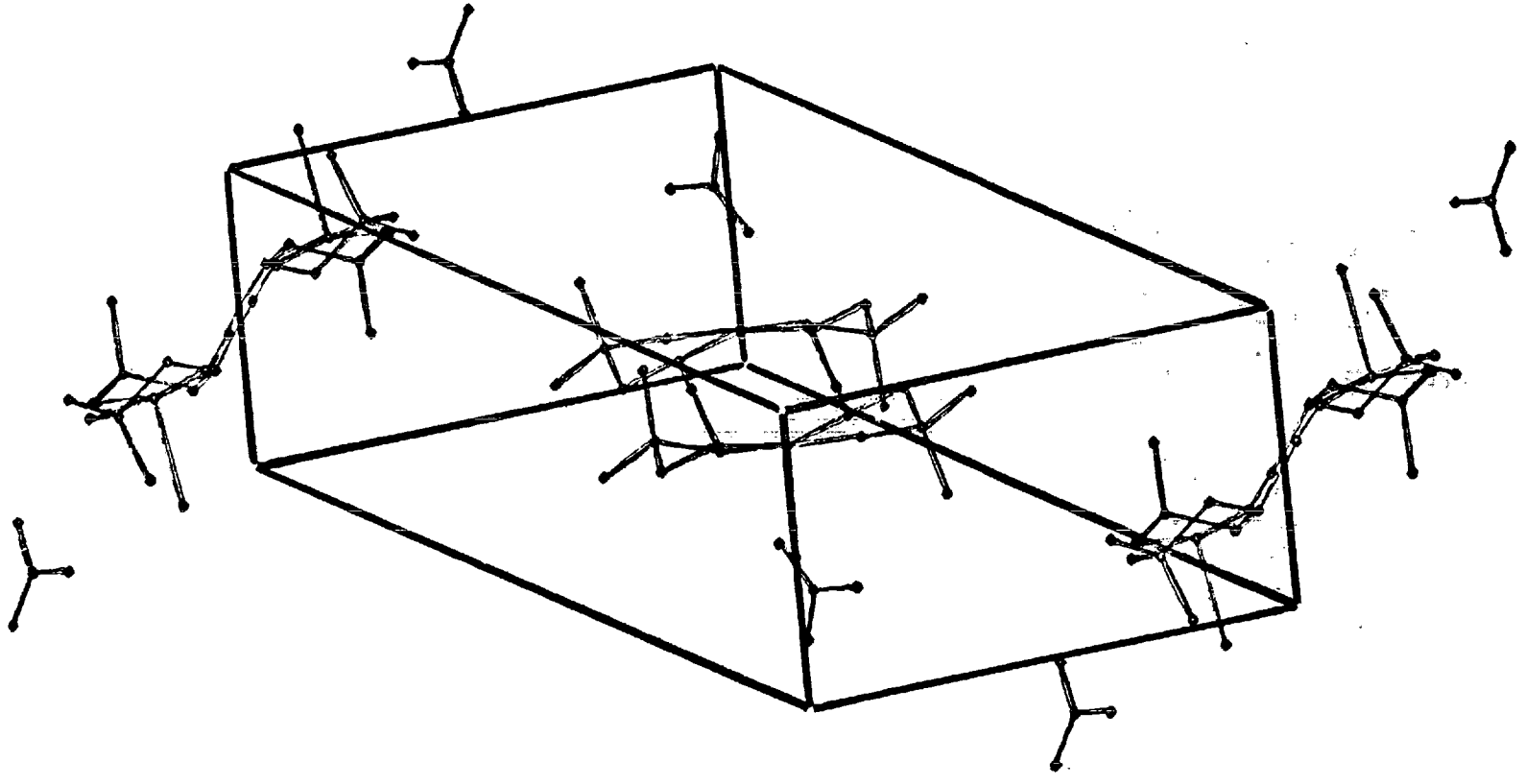


Figure 18. A Perspective View of the Crystal Packing of CuMep

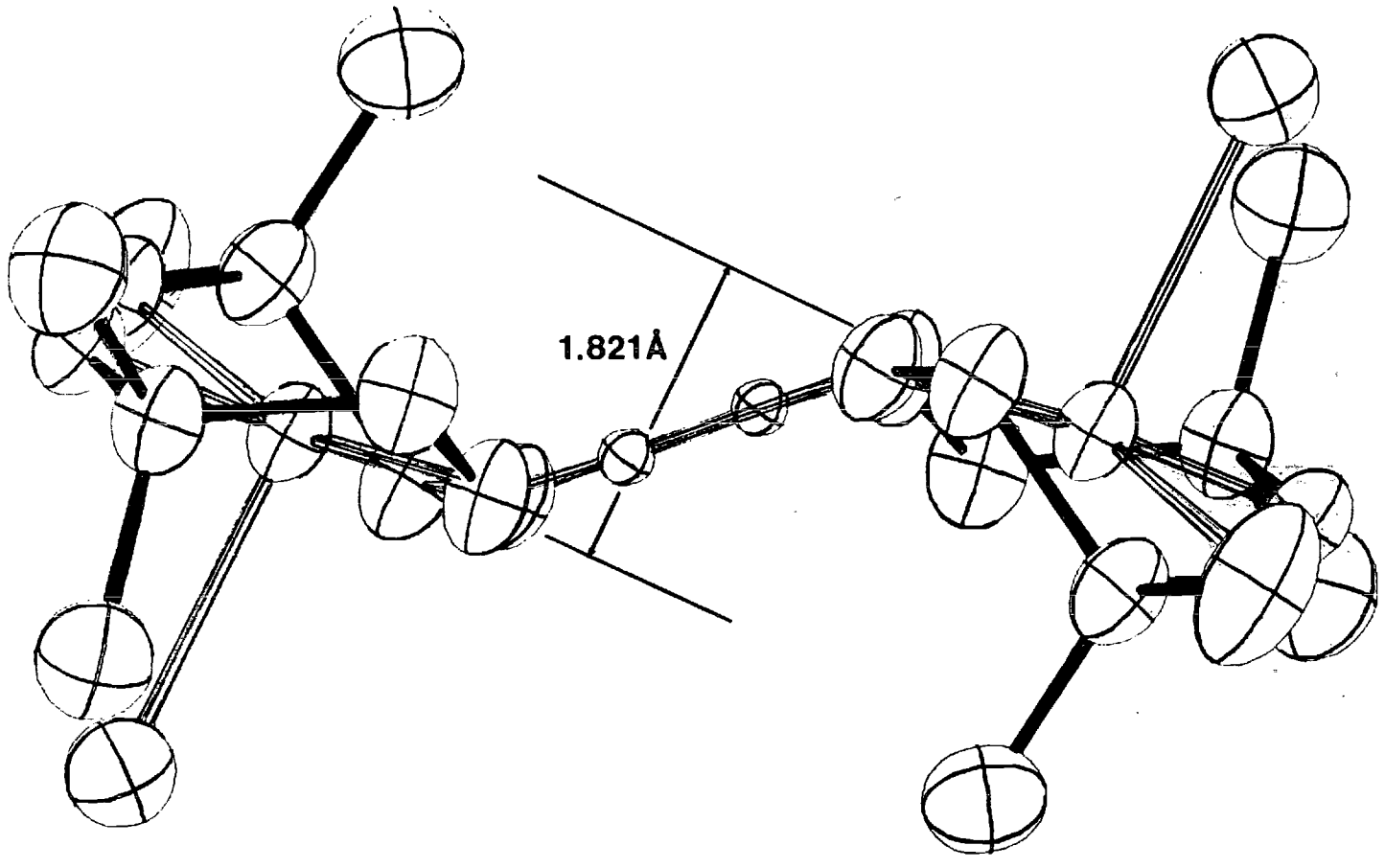


Figure 19. View of the Dinuclear Cation, $[Cu(Mep)(MepH)(H_2O)]_2^{2+}$, Showing the "Step" Arrangement

copper distance of 4.934(1)Å is slightly shorter. In this compound the eight-membered ring is slightly distorted with Cu-O2-O" and Cu-O1-O2" angles (where X and X" are related by the center of inversion at (-1/2, 0, 0)) of 117.2(1) and 130.6(1)°, respectively. The two basal coordination planes are separated by a distance of 1.821Å, Figure 19.

The nitrate anion appears to be associated with two amino groups by weak hydrogen bonds, Figure 18. N1-ON2 and N2-ON1 distances are 2.977(5) and 3.302(7)Å, respectively. N1-H2N1-ON2 and N2-H2N2-ON1 angles are 142(4) and 164(3)°, respectively.

Cu(ℓ-Eph)

Atomic coordinates for two sets of copper atoms were deduced from a three-dimensional Patterson synthesis and refined to give the initial residuals, R = 0.381 and R_w = 0.464. The remaining atoms were located by means of Fourier syntheses and least-squares refinements. A refinement using weighting scheme and isotropic temperature factors for 47 atoms converged with R = 0.206 and R_w = 0.206. Anisotropic thermal parameters for two sets of copper atoms, one set of chlorine atoms (anisotropic thermal parameters of other chlorine atoms were not refined) and carbon atoms whose thermal parameters were large, were introduced and further refinement reduced R to 0.107 and R_w to 0.103. Oxygens of two perchlorate anions and the oxygen of an uncoordinated water molecule were not refined. Two perchlorate anions were introduced as rigid groups and further refinements converged to the final values of R = 0.103 and R_w = 0.097. In the final cycle of refinement, the maximum parameter shift was 0.05σ (z coordinate of OW1). The major feature on a final difference Fourier

map was a peak about 1.5Å from the oxygen of the perchlorate group and the remaining residual electron density was located largely in the vicinity of the perchlorate groups. Final atomic parameters for 61 atoms (one oxygen of water molecule was not located), selected interatomic distances and angles are in Table 20, 21, and 22, respectively. Final calculated and observed structure factors are listed in the Appendix. The numbering scheme of atoms is shown in Figure 20. The dimeric unit is illustrated in Figure 21.

In the solution of the structure, space group $P3_1$ was first chosen. Refinements with the space group $P3_1$ gave the mirror image of the absolute configuration of ℓ-ephedrine determined previously.[22,48,49] Therefore, $P3_2$ was determined as the correct space group for this compound.

The structure of Cu(ℓ-Eph) consists of one dinuclear cation, $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2^{2+}$, two independent perchlorate anions, and two uncoordinated water molecules. (The oxygen of one water molecule was not refined.)

Each copper(II) atom shows square-planar coordination geometry and a cis-arrangement of two ℓ-ephedrine ligands. The copper-oxygen and copper-nitrogen distances are in the range of 1.89(1) to 2.05(1)Å and bond angles at copper range from 83.2(5) to 102.5(4)°.

The bis-chelated copper(II) complexes are associated into hydrogen-bonded dinuclear units (Figure 21). The oxygen-oxygen distances of hydrogen-bonds are 2.38(1) and 2.44(1)Å. The copper-copper distances are 4.849(4)Å. Cu1-O1-O4, Cu1-O2-O3, Cu2-O3-O2, and Cu2-O4-O1 angles are 120.7(6), 118.8(5), 121.9(5), and 118.1(5), respectively.

Table 20. Positional and Thermal Parameters for $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$*

Atom	x	y	z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu1	-.1257(1)	-.0070(1)	.3300	.0075(1)	.0058(1)	.0035(1)	.0018(1)	-.0001(1)	.0003(1)
Cu2	.0949(1)	.4116(1)	.3234(1)	.0054(1)	.0068(1)	.0035(1)	.0026(1)	.0002(1)	-.0001(1)
Cℓ1	-.3419(4)	-.4258(5)	.3359(4)	.0135(5)	.0129(5)	.0075(3)	.0037(4)	.0006(3)	-.0018(3)
Cℓ2	.2093(6)	-.4370(6)	.0948(3)	13.0 (2)					
O1	-.1394(8)	.1202(8)	.3565(4)	5.5 (2)					
O2	.0194(7)	.0992(7)	.2973(4)	5.4 (2)					
O3	.1327(7)	.2935(7)	.3351(4)	5.1 (2)					
O4	-.0595(7)	.2961(7)	.3063(4)	5.1 (2)					
OW1	.187 (2)	-.237 (2)	.267 (1)	19.6					
PO11	-.348	-.374	.374	21.7					
PO12	-.242	-.412	.316	21.7					
PO13	-.440	-.521	.312	21.7					
PO14	-.335	-.318	.285	21.7					
PO21	.094	-.493	.093	21.6					
PO22	.248	-.439	.147	21.6					
PO23	.251	-.501	.061	21.6					
PO24	.259	-.318	.079	21.6					
N1	-.289 (1)	-.105 (1)	.354 (1)	6.0 (3)					
N2	-.091 (1)	-.128 (1)	.309 (1)	6.0 (3)					
N3	.267 (1)	.521 (1)	.338 (1)	6.3 (3)					
N4	.035 (1)	.522 (1)	.313 (1)	4.9 (3)					
C11	-.249 (1)	.092 (1)	.382 (1)	5.7 (3)					
C12	-.304 (1)	-.043 (2)	.400 (1)	8.1 (4)					
C13	-.228 (1)	.174 (1)	.424 (1)	6.3 (4)					
C14	-.124 (1)	.235 (1)	.453 (1)	7.0 (4)					
C15	-.107 (2)	.314 (2)	.488 (1)	.024 (3)	.019 (2)	.004 (1)	.013 (2)	.000 (1)	-.002 (1)
C16	-.187 (2)	.350 (2)	.504 (1)	.020 (3)	.014 (2)	.007 (1)	.004 (2)	.003 (1)	-.001 (1)
C17	-.289 (3)	.296 (3)	.475 (1)	.032 (3)	.036 (4)	.006 (1)	.022 (3)	.010 (1)	.006 (1)
C18	-.317 (2)	.196 (2)	.434 (1)	.019 (2)	.017 (2)	.004 (1)	.012 (2)	.004 (1)	.002 (1)
C19	-.241 (2)	-.045 (1)	.451 (1)	.019 (2)	.013 (2)	.004 (1)	.004 (2)	-.001 (1)	.003 (1)

Table 20. (Continued)

Atom	x	y	z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
CN1	-.365 (1)	-.121 (2)	.310 (1)	.009 (2)	.023 (2)	.003 (1)	.005 (2)	-.001 (1)	.003 (1)
C21	.081 (1)	.046 (1)	.278 (1)	4.0 (3)					
C22	-.015 (1)	-.080 (1)	.262 (1)	6.9 (4)					
C23	.157 (1)	.116 (1)	.227 (1)	5.4 (3)					
C24	.153 (1)	.210 (1)	.210 (1)	6.9 (4)					
C25	.238 (2)	.276 (2)	.165 (1)	.016 (2)	.019 (2)	.003 (1)	.006 (2)	-.002 (1)	.001 (1)
C26	.304 (2)	.237 (2)	.147 (1)	.013 (2)	.024 (3)	.005 (1)	.001 (2)	-.003 (1)	.001 (1)
C27	.309 (2)	.142 (2)	.170 (1)	.015 (2)	.028 (3)	.002 (1)	.008 (2)	.001 (1)	.001 (1)
C28	.238 (1)	.083 (2)	.208 (1)	.010 (2)	.019 (3)	.002 (1)	.006 (2)	-.001 (1)	-.001 (1)
C29	-.087 (1)	-.088 (1)	.213 (1)	.017 (2)	.010 (2)	.002 (1)	.004 (1)	-.002 (1)	-.001 (1)
CN2	-.032 (2)	-.152 (2)	.353 (1)	.020 (2)	.017 (2)	.004 (1)	.012 (2)	-.001 (1)	.001 (1)
C31	.252 (1)	.331 (1)	.341 (1)	4.0 (3)					
C32	.302 (1)	.455 (1)	.373 (1)	7.0 (4)					
C33	.268 (1)	.246 (1)	.374 (1)	5.3 (3)					
C34	.185 (1)	.171 (1)	.414 (1)	6.0 (4)					
C35	.197 (2)	.087 (1)	.439 (1)	.016 (2)	.010 (2)	.003 (1)	.007 (2)	.001 (1)	-.001 (1)
C36	.289 (2)	.073 (2)	.433 (1)	.020 (3)	.011 (2)	.006 (1)	.007 (2)	.005 (1)	.001 (1)
C37	.372 (2)	.147 (2)	.394 (1)	.026 (2)	.026 (2)	.005 (1)	.022 (2)	-.007 (1)	-.006 (1)
C38	.359 (1)	.228 (1)	.369 (1)	.009 (1)	.013 (2)	.006 (1)	.009 (1)	-.003 (1)	-.002 (1)
C39	.253 (1)	.446 (1)	.429 (1)	.011 (2)	.008 (2)	.004 (1)	.003 (1)	.000 (1)	-.002 (1)
CN3	.325	.564 (1)	.287 (1)	.011 (2)	.014 (2)	.004 (1)	.004 (1)	.002 (1)	.004 (1)
C41	-.138 (1)	.337 (1)	.300 (1)	5.4 (4)					
C42	-.064 (1)	.466 (1)	.281 (1)	6.0 (4)					
C43	-.238 (1)	.264 (1)	.268 (1)	5.1 (3)					
C44	-.230 (2)	.192 (2)	.228 (1)	8.2 (4)					
C45	-.328 (2)	.117 (2)	.200 (1)	.015 (2)	.018 (2)	.006 (1)	.011 (2)	-.001 (1)	-.003 (1)
C46	-.423 (2)	.111 (2)	.209 (1)	.019 (3)	.014 (2)	.003 (1)	.005 (2)	.001 (1)	.001 (1)
C47	-.443 (1)	.174 (2)	.249 (1)	.009 (2)	.026 (3)	.004 (1)	.008 (2)	-.001 (1)	.001 (1)
C48	-.346 (1)	.261 (2)	.278 (1)	.011 (1)	.019 (2)	.003 (1)	.009 (1)	-.001 (1)	.003 (1)

Table 20. (Continued)

Atom	x	y	z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C49	-.025 (2)	.462 (1)	.217 (1)	.020 (2)	.012 (1)	.003 (1)	.006 (1)	.001 (1)	.002 (1)
CN4	.013 (2)	.549 (2)	.364 (1)	.026 (2)	.017 (2)	.002 (1)	.015 (2)	.000 (1)	.000 (1)

*The form of thermal ellipsoid expression is exp $[-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - \beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl]$. Oxygens of perchlorate anions are refined as groups.

Table 21. Interatomic Distances (Å) for $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$

Atoms	Distance	Atoms	Distance
Cu1-Cu2	4.849(4)	C23-C24	1.36(2)
O1-O4	2.38(1)	C24-C25	1.52(3)
O2-O3	2.44(1)	C25-C26	1.31(3)
Cu1-O1	1.91(1)	C26-C27	1.42(3)
Cu1-O2	1.92(1)	C27-C28	1.30(2)
Cu1-N1	1.99(1)	C28-C23	1.43(2)
Cu1-N2	1.97(1)	C22-C29	1.51(2)
Cu2-O3	1.92(1)	N2-CN2	1.47(2)
Cu2-O4	1.89(1)	O3-C31	1.41(1)
Cu2-N3	2.06(1)	C31-C32	1.64(2)
Cu2-N4	2.00(1)	C32-N2	1.48(2)
O1-C11	1.46(2)	C31-C33	1.52(2)
C11-C12	1.63(2)	C33-C34	1.45(2)
C12-N1	1.49(2)	C34-C35	1.36(2)
C11-C13	1.43(2)	C35-C36	1.34(2)
C13-C14	1.41(2)	C36-C37	1.43(3)
C14-C15	1.29(2)	C37-C38	1.33(3)
C15-C16	1.43(3)	C38-C33	1.36(2)
C16-C17	1.39(4)	C32-C39	1.53(2)
C17-C18	1.56(4)	N3-CN3	1.43(2)
C18-C13	1.38(2)	O4-C41	1.41(2)
C12-C19	1.51(2)	C41-C42	1.56(2)
N1-CN1	1.42(2)	C42-N2	1.40(2)
O2-C21	1.41(1)	C41-C43	1.44(2)
C21-C22	1.58(2)	C43-C44	1.40(2)
C22-N2	1.46(2)	C44-C45	1.38(2)
C21-C23	1.59(2)	C45-C46	1.25(2)
		C46-C47	1.40(3)
C11-PO11	1.19(1)	C47-C48	1.43(3)
C11-PO12	1.36(1)	C48-C43	1.46(2)
C11-PO13	1.42(1)	C42-C49	1.67(3)
C11-PO14	1.88(1)	N4-CN4	1.39(2)
C12-PO21	1.34(1)		
C12-PO22	1.40(1)		
C12-PO23	1.49(1)		
C12-PO24	1.45(1)		

Table 22. Interatomic Angles (Degrees) for $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$

Atoms	Angle	Atoms	Angle
O1-Cu1-O2	89.9(4)	O2-C21-C22	105(1)
O1-Cu1-N1	85.7(4)	O2-C21-C23	110(1)
O1-Cu1-N2	171.8(5)	C21-C22-C23	106(1)
O1-Cu1-N1	168.9(5)	C21-C22-C29	116(1)
O2-Cu1-N2	85.8(4)	C22-N2-CN2	112(1)
N1-Cu1-N2	99.7(5)	N2-C22-C29	109(1)
Cu1-O1-C11	116.5(8)	C23-C24-C25	114(2)
Cu1-O1-O4	120.2(5)	C24-C25-C26	118(2)
Cu1-O2-C21	113.4(7)	C25-C26-C27	124(2)
Cu1-O2-O3	119.1(5)	C26-C27-C28	119(2)
Cu1-N1-C12	105.3(9)	C27-C28-C23	119(2)
Cu1-N1-CN1	110.1(10)	C28-C23-C24	124(2)
Cu1-N2-C22	104.2(9)	O3-Cu2-O4	89.6(4)
Cu1-N2-CN2	110.2(11)	O3-Cu2-N3	83.4(4)
O1-C11-C12	104(1)	O3-Cu2-N4	170.9(5)
O1-C11-C13	109(1)	O4-Cu2-N3	172.9(4)
C11-C12-N1	107(1)	O4-Cu2-N4	85.0(4)
C11-C12-C19	107(1)	N3-Cu2-N4	101.9(5)
C12-N1-CN1	113(1)	Cu2-O3-C31	115.8(7)
N1-C12-C19	114(2)	Cu2-O3-O2	121.5(5)
C13-C14-C15	123(2)	Cu2-O4-C41	114.9(8)
C14-C15-C16	127(2)	Cu2-O4-O1	118.6(5)
C15-C16-C17	113(2)	Cu2-N3-C32	106.0(9)
C16-C17-C18	122(2)	Cu2-N3-CN3	106.8(10)
C17-C18-C13	116(2)	Cu2-N4-C42	106.0(9)
C18-C13-C14	119(2)	Cu2-N4-CN4	109.5(10)
O3-C31-C32	104(1)	PO11-C11-PO12	124(1)
O3-C31-C33	110(1)	PO11-C11-PO13	123(1)
C31-C32-N3	121(1)	PO11-C11-PO14	94(1)
C31-C32-C39	109(1)	PO12-C11-PO13	112(1)
C32-N3-CN3	119(1)	PO12-C11-PO14	89(1)
N3-C32-C39	109(1)	PO13-C11-PO14	94(1)
C33-C34-C35	121(1)	PO21-C12-PO22	111(1)
C34-C35-C36	124(2)	PO21-C12-PO23	109(1)
C35-C36-C37	116(2)	PO21-C12-PO24	111(1)
C36-C37-C38	120(2)	PO22-C12-PO23	106(1)
C37-C38-C33	126(2)	PO22-C12-PO24	108(1)
C38-C33-C34	113(1)	PO23-C12-PO24	112(1)
O4-C41-C42	107(1)	N4-C42-C49	109(1)
O4-C41-C43	114(1)	C43-C44-C45	119(2)
C41-C42-N4	109(1)	C44-C45-C46	121(2)
C41-C42-C49	106(1)	C45-C46-C47	126(2)
C42-N4-CN4	112(1)	C46-C47-C48	118(2)
		C47-C48-C43	114(2)
		C48-C43-C44	121(1)

Table 23. Least Square Planes Within the Molecule $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$[ab]

Atom	Deviation (Å)	Atom	Deviation (Å)
(a) Plane involving four atoms (O1, O2, N1, and N2) coordinated to Cu1			
Equation: $-0.443x + 0.011y - 0.897z - 6.546 = 0$			
O1	.144	N2	.112
O2	-.115	Cu1	.047
N1	-.151		
(b) Plane involving four atoms (O3, O4, N3, and N4) coordinated to Cu2			
Equation: $0.221x + 0.039y - 0.974z - 7.904 = 0$			
O3	.053	N4	.059
O4	-.063	Cu2	.029
N3	-.050		

[a]Direction cosines of the planes refer to the orthogonal axis system a,b,c*.

[b]All atoms weighted at unity.

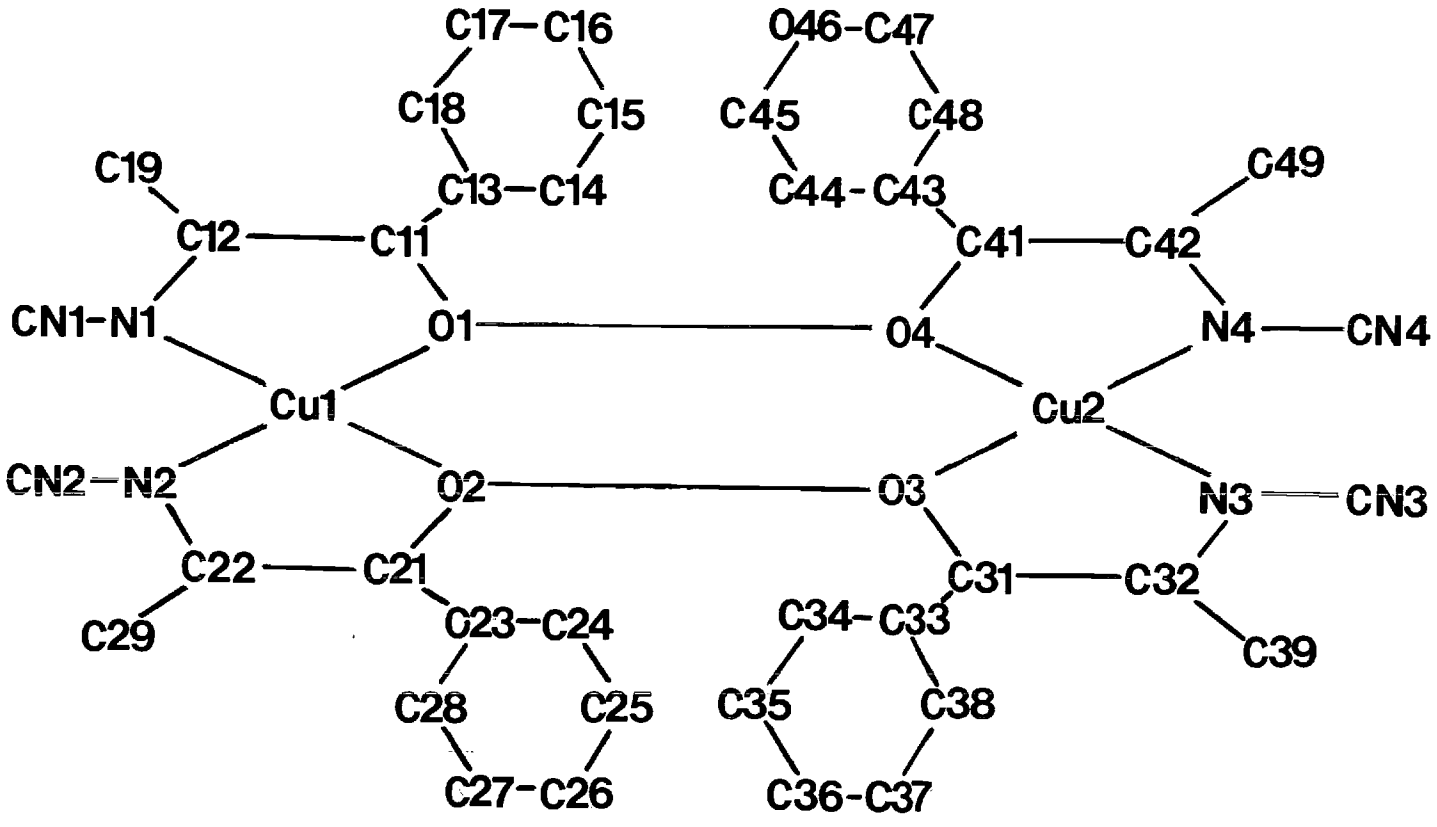


Figure 20. The Numbering Scheme of Atoms in Cu(ℓ-Eph)

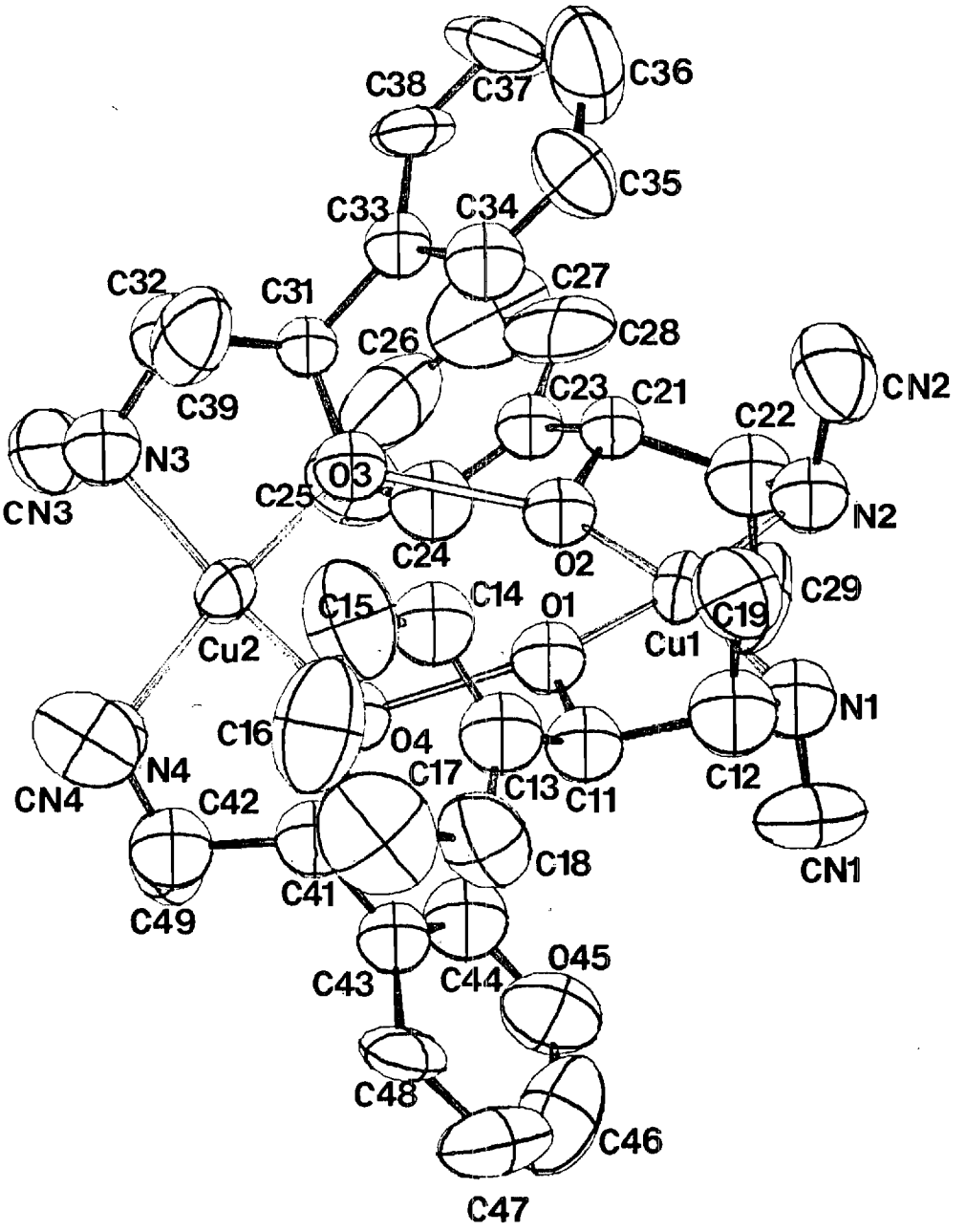


Figure 21. Structure of the Dinuclear Hydrogen-bonded Cation, $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2^{2+}$

An interesting feature of this structure is that the two coordination planes around copper are not parallel, due to the steric hindrance of the phenyl groups; the dihedral angle of the two coordination planes is about 40°.

CuDme

Two copper atoms and an oxygen atom were located from a three-dimensional Patterson synthesis. After two cycles of full-matrix least-squares refinement of coordinates and isotropic temperature factors for these atoms, values for R of 0.45 and R_w of 0.50 were obtained. One chlorine atom and several oxygen, nitrogen, and/or carbon atoms were located by means of Fourier syntheses and least-squares refinement, but the R value was not reduced significantly. The remaining chlorine atoms were not observed in the electron density map.

The problems of refining this structure are possibly caused by the crystal being twinned, the crystal containing disordered groups, or the collected data being poor. The portion of the structure located is a linear trimer of copper atoms with bridging oxygens.

CoDeta

Two cobalt atoms and one oxygen atom were located from a three-dimensional Patterson synthesis. Three cycles of full-matrix least-squares refinement of the coordinates and isotropic temperature factors for these atoms resulted in R of 0.367 and R_w of 0.39. The remaining oxygen, nitrogen, carbon, and chlorine atoms were located by means of subsequent difference Fourier calculation and least-squares refinement. A refinement using a weighting scheme based on counting statistics

($w = 4I/\sigma^2(I)$) and using isotropic temperature factors for all non-hydrogen atoms converged with R = 0.109 and R_w = 0.106. Anisotropic thermal parameters were introduced and further refinements reduced R to 0.056 and R_w to 0.049. The 29 hydrogen atoms were located as principal features on an electron density map; in subsequent refinements, the hydrogen coordinates were varied but the hydrogen thermal parameters were fixed at 5.0. The positional parameters of five hydrogens which are bonded to C21, C24, and C33 did not refine well and were fixed. The refinement converged to the final values of R = .045 and R_w = .035. In the final cycle of refinement, the maximum parameter shift was 0.43σ (x coordinate of HN3). The major feature on a final difference Fourier map was a peak of $0.64e\text{Å}^{-3}$, approximately 0.9Å from Co1; this compares to values of approximately 3.5 and $0.5e\text{Å}^{-3}$ for typical carbon and hydrogen atoms in this structure. Final atomic parameters are listed in Table 24; final calculated and observed structure factors are listed in the Appendix. Selected bond distances and bond angles are tabulated in Tables 25 and 26, respectively. The tetrameric unit is illustrated in Figure 23.

The structure of this compound is best represented by the formula $[\ Co(II)Co(III)(Deta)_2(DetaH_2)]_2(ClO_4)_2$. The skeleton of the tetrameric unit shown in Figure 22, consists of portions of two adjoining cubes in which alternate corners are oxygen and cobalt; there is a center of symmetry on the interface between the two cubes, with two symmetry-related extreme corner cobalt atoms removed. There remain four octahedral cobalts with two μ_3-alkoxide and two μ-alkoxide bridges coordinated to each of the interface cobalts (Co2 and Co2′), and two μ-alkoxide and one μ_3-alkoxide bridges coordinated to the remaining (extreme) cobalts (Co1 and

Table 24. Positional and Thermal Parameters for $[Co_2(Deta)_2(DetaH_2)]_2(ClO_4)_2$*

Atom	x	y	z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co1	.09258(7)	-.02618(3)	.20073(4)	.01142(10)	.00174(2)	.00276(3)	.00058(4)	.00181(5)	.00004(3)
Co2	.14060(7)	.06711(3)	.02038(4)	.00992(10)	.00222(2)	.00310(3)	-.00028(4)	.00223(5)	-.00003(2)
Cℓ	.4018(2)	-.3451(1)	.0861(1)	.0179(3)	.0032(1)	.0046(1)	-.0001(1)	.0017(1)	.0000(1)
P01	.5667(7)	-.3553(4)	.1066(7)	.0205(10)	.0081(3)	.0368(11)	.0036(8)	.0103(8)	.0076(5)
P02	.3416(6)	-.2830(3)	.0157(3)	.0273(8)	.0058(2)	.0104(4)	.0020(4)	.0048(5)	.0033(2)
P03	.3164(7)	-.4128(3)	.0408(3)	.0460(14)	.0058(2)	.0091(3)	-.0074(5)	.0044(6)	-.0015(2)
P04	.3735(10)	-.3332(3)	.1796(4)	.0794(24)	.0074(3)	.0084(4)	.0075(6)	.0147(8)	.0008(2)
011	-.0424(3)	.0338(1)	.0842(2)	.0098(5)	.0019(1)	.0034(2)	.0006(2)	.0023(2)	.0004(1)
012	-.0810(4)	-.0624(2)	.2460(2)	.0175(6)	.0025(1)	.0041(2)	-.0012(2)	.0045(3)	-.0003(1)
021	.2639(3)	.0136(2)	.1619(2)	.0095(5)	.0034(1)	.0042(2)	.0009(2)	.0017(2)	.0004(1)
022	.0499(4)	-.1097(2)	.1059(2)	.0171(6)	.0018(1)	.0038(2)	.0014(2)	.0013(3)	-.0009(1)
031	.3059(4)	.0705(2)	-.0595(2)	.0147(6)	.0041(1)	.0051(2)	-.0020(3)	.0044(3)	-.0013(2)
032	.1723(8)	.2969(3)	.1957(4)	.0499(16)	.0037(2)	.0081(3)	.0038(4)	.0007(4)	.0002(2)
N1	.0998(5)	.0632(2)	.2910(3)	.0138(9)	.0023(1)	.0040(2)	-.0003(3)	.0050(4)	-.0007(2)
N2	.2599(5)	-.0916(2)	.3005(3)	.0196(9)	.0030(2)	.0034(2)	.0016(3)	.0036(6)	-.0015(2)
N3	.2772(6)	.1755(2)	.0876(3)	.0198(7)	.0034(2)	.0053(3)	-.0021(3)	.0027(4)	-.0003(2)
C11	-.1233(6)	.0914(3)	.1204(4)	.0140(9)	.0020(2)	.0053(3)	.0016(3)	.0046(5)	.0005(2)
C12	-.0028(7)	.1251(3)	.2221(4)	.0192(11)	.0017(2)	.0053(4)	.0010(3)	.0053(5)	.0001(2)
C13	.0358(7)	.0360(3)	.3736(3)	.0215(11)	.0031(2)	.0031(3)	-.0001(4)	.0039(5)	-.0004(2)
C14	-.1145(7)	-.0111(3)	.3184(4)	.0219(12)	.0031(2)	.0052(4)	-.0021(4)	.0077(6)	-.0006(2)
C21	.4125(7)	-.0247(4)	.2114(5)	.0145(11)	.0057(3)	.0098(5)	.0054(5)	.0044(6)	.0021(3)
C22	.4182(8)	-.0546(4)	.3153(5)	.0156(12)	.0046(3)	.0085(5)	.0025(5)	-.0012(6)	.0013(3)
C23	.2398(9)	-.1697(3)	.2546(4)	.0301(16)	.0023(2)	.0057(4)	.0032(5)	-.0008(7)	.0004(2)
C24	.1266(14)	-.1732(4)	.1526(5)	.0747(44)	.0032(3)	.0087(6)	.0094(10)	-.0126(13)	-.0026(4)
C31	.4062(9)	.1376(4)	-.0386(5)	.0191(12)	.0061(3)	.0068(4)	-.0055(5)	.0066(6)	-.0025(3)
C32	.4377(8)	.1599(5)	.0740(13)	.0193(13)	.0063(3)	.0075(5)	-.0051(6)	.0052(6)	-.0020(3)
C33	.2149(10)	.2515(4)	.0452(5)	.0362(18)	.0040(3)	.0079(5)	-.0032(6)	.0034(8)	-.0007(3)
C34	.0963(12)	.2858(4)	.0875(5)	.0409(21)	.0042(3)	.0077(5)	.0019(7)	.0050(9)	.0010(3)
H031	.236(6)	.073(3)	-.122(4)						
H032	.147(6)	.331(3)	.211(4)						
HN1	.194(7)	.087(3)	.322(4)						
HN2	.258(6)	-.094(3)	.366(4)						

Table 24. (Continued)

Atom	x	y	z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
HN3	.319(6)	.180(3)	.163(4)						
HA11	-.229(7)	.066(3)	.123(4)						
HB11	-.141(6)	.128(3)	.073(4)						
HA12	.065(6)	.161(3)	.204(4)						
HB12	-.059(6)	.155(3)	.259(4)						
HA13	.137(7)	.008(3)	.423(4)						
HB13	.013(6)	.082(3)	.409(4)						
HA14	-.211(7)	.028(3)	.284(4)						
HB14	-.147(6)	-.037(3)	.367(4)						
HA21	.434(6)	-.058(3)	.167(4)						
HB21	.502	.013	.224						
HA22	.425(6)	-.014(3)	.366(4)						
HB22	.487(7)	-.084(3)	.341(4)						
HA23	.188(6)	-.196(3)	.311(4)						
HB23	.309(7)	-.192(3)	.287(4)						
HA24	.057	-.211	.146						
HB24	.198	-.186	.110						
HA31	.351(6)	.180(3)	-.087(4)						
HB31	.511(7)	.129(3)	-.045(4)						
HA32	.522(7)	.204(3)	.094(4)						
HB32	.501(7)	.114(3)	.125(4)						
HA33	.309	.286	.063						
HB33	.166	.249	-.030						
HA34	-.022(7)	.240(3)	.063(4)						
HB34	.043(6)	.336(3)	.047(4)						

*The form of the thermal ellipsoid expression is exp $[-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}\ell^2 - 2\beta_{12}hk - 2\beta_{13}h\ell - 2\beta_{23}k\ell]$.

All hydrogen atoms were assigned isotropic thermal parameters of 5.0. Positional parameters of HB21, HA24, HB24, HA33 and HB33 were not refined.

Table 25. Interatomic Distances for $[Co_2(Deta)_2(DetaH_2)]_2(C\ell O_4)_2$[a,b]

Atoms	Distance (Å)	Atoms	Distance (Å)
Co1-Co2	3.096(2)	C23-C24	1.380(7)
Co1-Co2'	3.037(3)	C24-O22	1.328(7)
Co1-Co1'	5.176(4)	O31-C31	1.426(6)
Co2-Co2'	3.289(3)	C31-C32	1.504(8)
Co1-O11	1.904(3)	C32-N3	1.507(8)
Co1-O12	1.940(3)	N3-C33	1.466(8)
Co1-O21	1.893(3)	C33-C34	1.484(10)
Co1-O22	1.888(3)	C34-O32	1.388(8)
Co1-N1	1.968(4)		
Co1-N2	1.957(4)	Cℓ-PO1	1.377(6)
Co2-O11	2.161(3)	Cℓ-PO2	1.412(4)
Co2-O11'	2.225(3)	Cℓ-PO3	1.412(4)
Co2-O21	2.053(3)	Cℓ-PO4	1.397(5)
Co2-O22'	2.045(3)		
Co2-O31	2.103(4)	O31-HO31	.85(5)
Co2-N3	2.241(4)	O32-HO32	.69(5)
O11-C11	1.416(5)	N1-HN1	.95(5)
C11-C12	1.517(7)	N2-HN2	.90(5)
C12-N1	1.494(6)	N3-HN3	.88(5)
N1-C13	1.503(6)	C11-HA11	1.04(5)
C13-C14	1.498(7)	C11-HB11	.88(5)
C14-O12	1.436(6)	C12-HA12	.95(5)
O21-C21	1.395(6)	C12-HB12	.98(5)
C21-C22	1.489(9)	C13-HA13	1.02(5)
C22-N2	1.473(8)	C13-HB13	.99(5)
N2-C23	1.479(7)	C14-HA14	1.05(5)
C14-HB14	.93(5)		
C21-HA21	.91(5)		
C21-HB21	.98		
C22-HA22	.97(5)		
C22-HB22	.77(5)		
C23-HA23	1.13(5)		
C23-HB23	.71(5)		
C24-HA24	.88		
C24-HB24	1.02		
C31-HA31	.99(5)		
C31-HB31	.97(5)		
C32-HA32	1.03(5)		
C32-HB32	1.08(5)		
C33-HA33	.98		
C33-HB33	.95		
C34-HA34	1.25(5)		
C34-HB34	1.04(6)		
O32-O12''	2.782(5)		

[a] X and X' are related by the inversion operation.

[b] X and X'' are related by the 2-fold and translation operation.

Table 26. Interatomic Angles for $[Co_2(Deta)_2(DetaH_2)]_2(C\ell O_4)_2$[a,b]

Atoms	Angle	Atoms	Angle
	(Degrees)		(Degrees)
O11-Co1-O12	97.1(1)	O21-Co2-N3	88.9(2)
O11-Co1-O21	83.1(1)	O22'-Co2-O31	93.4(2)
O11-Co1-O22	86.9(1)	O22'-Co2-N3	100.7(2)
O11-Co1-N1	87.4(1)	O31-Co2-N3	79.8(2)
O11-Co1-N2	167.2(2)	Co1-O11-Co2	99.0(1)
O12-Co1-O21	176.9(1)	Co1-O11-Co2'	94.4(1)
O12-Co1-O22	89.1(1)	Co1-O11-C11	109.7(2)
O12-Co1-N1	84.8(1)	Co2-O11-Co2'	97.2(1)
O12-Co1-N2	93.7(2)	Co2-O11-C11	119.2(3)
O21-Co1-O22	94.0(1)	Co2'-O11-C11	131.0(3)
O21-Co1-N1	92.1(2)	Co1-O12-C14	113.3(3)
O21-Co1-N2	86.5(2)	Co1-O21-Co2	103.3(2)
O22-Co1-N1	171.1(2)	Co1-O21-C21	109.7(3)
O22-Co1-N2	86.3(2)	Co2-O21-C21	112.5(3)
N1-Co1-N2	100.5(2)	Co1-O22-Co2'	103.3(1)
O11-Co2-O11'	82.8(1)	Co1-O22-C24	112.0(3)
O11-Co2-O21	73.4(1)	Co2'-O22-C24	144.8(4)
O11-Co2-O22'	86.5(1)	Co2-O31-C31	114.2(3)
O11-Co2-O31	164.9(1)	Co1-N1-C12	107.7(3)
O11-Co2-N3	115.1(1)	Co1-N1-C13	106.4(3)
O11'-Co2-O21	100.9(1)	C12-N1-C13	113.1(4)
O11'-Co2-O22'	75.2(1)	Co1-N2-C22	105.5(3)
O11'-Co2-O31	82.5(1)	Co1-N2-C23	107.4(3)
O11'-Co2-N3	100.7(2)	C22-N2-C23	114.9(5)
O21-Co2-O22'	159.9(1)	Co2-N3-C32	100.4(4)
O21-Co2-O31	105.8(1)	Co2-N3-C33	122.2(4)
C32-N3-C33	110.1(5)		
O11-C11-C12	108.8(4)	PO1-Cℓ-PO2	109.9(3)
C11-C12-N1	110.5(4)	PO1-Cℓ-PO3	109.2(4)
N1-C13-C14	107.2(4)	PO1-Cℓ-PO4	110.9(5)
C13-C14-O12	108.8(4)	PO2-Cℓ-PO3	109.7(3)
O21-C21-C22	109.1(5)	PO2-Cℓ-PO4	111.0(3)
C21-C22-N2	108.6(5)	PO3-Cℓ-PO4	106.2(4)
N2-C23-C24	113.3(4)	O32-HO32-O11"	176 (6)
C23-C24-O22	119.7(5)		
O31-C31-C32	106.5(5)		
C31-C32-N3	109.8(5)		
N3-C33-C34	115.0(6)		
C33-C34-O32	109.5(7)		

[a] X and X' are related by the inversion operation.

[b] X and X" are related by the 2-fold and translation operation.

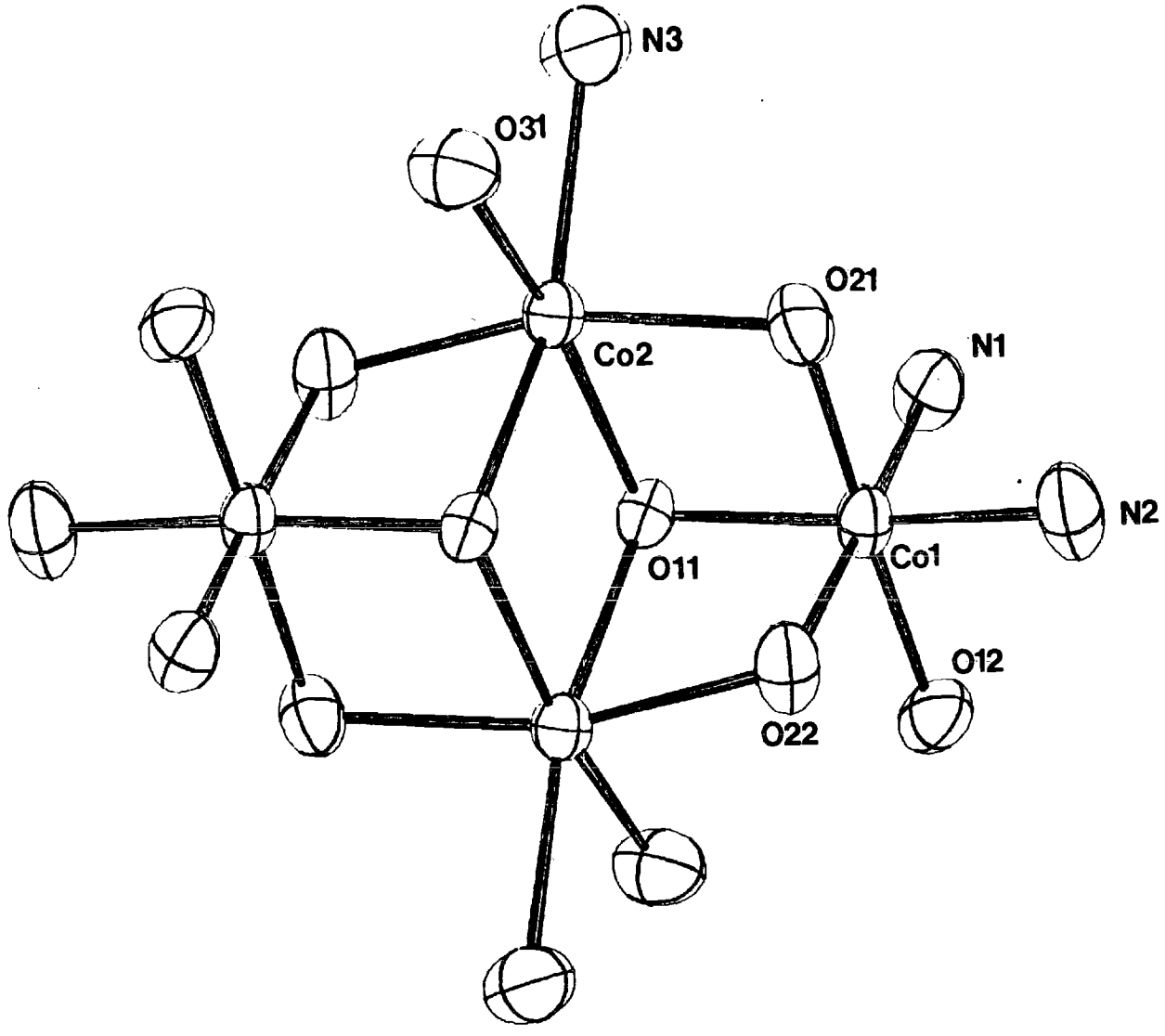


Figure 22. The Arrangement of the Cobalt Atoms and the Bridging Alkoxide Oxygen Atoms of CoDeta

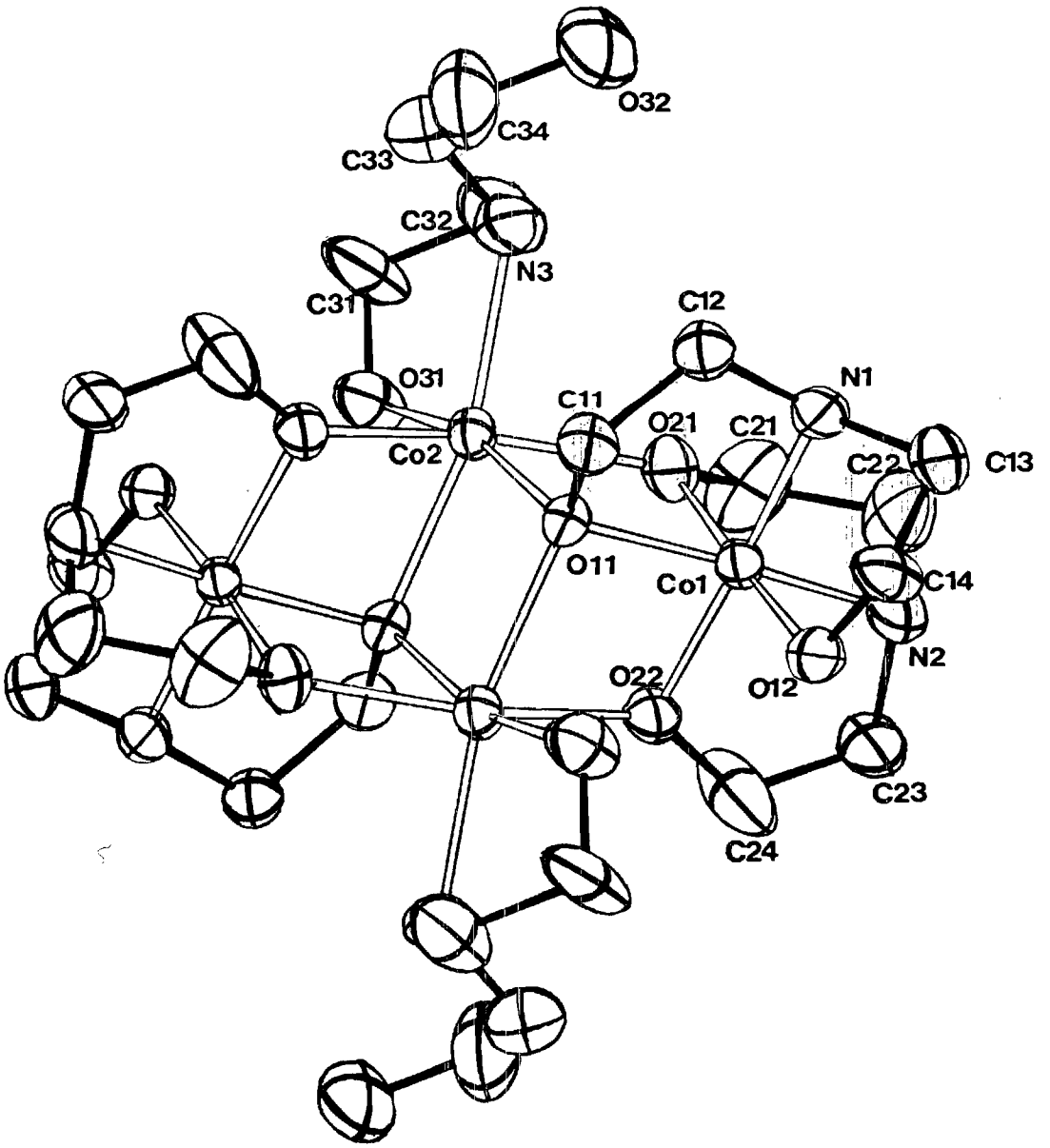


Figure 23. Structure of the Tetrameric Cation, $[Co_2(Deta)_2(DetaH_2)]_2^{2+}$

Co1′). The octahedral coordination of the Co1 atom is provided by two tridentate 2,2′-dihydroxydiethylamine dianion and consists of two amine nitrogen atoms (in cis positions) and four alkoxide oxygen atoms with the two oxygen atoms from one ligand also in cis positions. The average Co-N distance is 1.962Å and the four Co-O distances are between 1.88-1.94Å. The severely distorted octahedral coordination of the Co2 atom consists of one amine nitrogen atom, two μ_3-alkoxide oxygen atoms, two μ-alkoxide oxygen atoms, and one alcohol oxygen atom. The cobalt-coordinating atom distances are a Co-N of 2.241(4)Å, two Co-O's of 2.161(3) and 2.225(3)Å, two Co-O's of 2.053(3) and 2.045(3)Å, and a Co-O of 2.103(4)Å, respectively. All of these bond distances are longer than the corresponding bond distances for Co1. All of the nitrogen and oxygen atoms of two dianionic 2,2′-dihydroxydiethylamine ligands are coordinated to Co1, whereas the remaining symmetrically independent 2,2′-dihydroxydiethylamine ligand coordinated to Co2 has one uncoordinated alcohol oxygen atom. This alcohol oxygen atom is associated with one of the coordinated alkoxide oxygens, O12" (X and X" are related by twofold screw operation) by a weak hydrogen bond. O32-O12" and O32-HO32 distances are 2.782(5) and 0.69(5)Å. O32-HO32-O12" angle is 176(6)°. Tetramers are connected into chains in the b direction by this type of hydrogen bond.

$CuPIPA \cdot 2H_2O$

Atomic coordinates for copper, two oxygen atoms, and two nitrogen atoms were deduced from a three-dimensional Patterson synthesis and refined to give the initial residuals, $R = 0.33$ and $R_w = 0.41$. The remaining atoms were located by means of Fourier syntheses and least-squares

refinements. A refinement using a weighting scheme based on counting statistics ($w = 4I/\sigma^2(I)$) and isotropic temperature factors for all non-hydrogen atoms converged with $R = 0.109$ and $R_w = 0.139$. Anisotropic thermal parameters were introduced and further refinement reduced R to 0.090 and R_w to 0.092. The 12 principal faces of the crystal were identified as the following (distance in millimeters from the center of the crystal to the face is given in parentheses): {111} (0.11), {100} (0.05), and {001} (0.18). Absorption corrections, calculated by the gaussian quadrature method, were applied; corrections on F^2 ranged from 1.22 to 1.43. Refinement with the absorption-corrected data set, after deletion of several reflections which had erroneous scans due to instrumental malfunctions, reduced R to 0.062 and R_w to 0.051. The 14 hydrogen atoms were located as the principal features on an electron density map; in subsequent refinements, the hydrogen coordinates were varied but the hydrogen thermal parameters were fixed at the values of the corresponding carbon atoms prior to conversion to the anisotropic form. These refinements converged to give $R = 0.056$ and $R_w = 0.044$.

Examination of thermal ellipsoids for propyl carbon atoms C1 and C2 gave strong indications of either disorder or severe libration approximately normal to the coordination plane (approximately normal to the b axis). A difference electron density map revealed two distinct maxima separated by ca. 0.6Å about the refined C2 position and a slightly elongated streak of electron density about C1. Thus, in further refinements two partial atoms, C2A and C2B, were refined with occupancies α and $1 - \alpha$ rather than a single atom of occupancy 1.0. Nearly equal occupancy factors, 0.52 and 0.48, were obtained for C2A and C2B, respectively. The refinements

converged to final values of $R = 0.043$ and $R_w = 0.033$. Because of the success of the refinement and the normalcy of the thermal parameters for the other atoms, it is considered unlikely that the problem with C2 and C1 is due to ambiguity in the space group determination (i.e., Cc vs. C2/c) rather than to a genuine twofold static disorder. In the final cycle of refinement, the maximum parameter shift was 0.1σ (y coordinate for H103). The major feature on a final difference Fourier map was a peak of 0.48e $Å^{-3}$ ca. 2Å from O3; this compares to values of ca. 5.0 and $0.8eÅ^{-3}$ for typical carbon and hydrogen atoms in this structure. Final atomic parameters are listed in Table 27. Final calculated and observed structure factors are listed in the Appendix.

The structure of $CuPIPA \cdot 2H_2O$ is best represented by the formula $[Cu(PIPA)(H_2O)]_2 \cdot 2H_2O$. The dimeric molecular units, with crystallographic twofold symmetry, and the waters of crystallization linked by weak hydrogen bonding into an infinite two-dimensional network. The structure of the dimeric unit is illustrated in Figure 24 and the crystal packing is illustrated in Figure 25; selected interatomic distances and angles are presented in Tables 28 and 29.

Each copper atom has a distorted tetragonal-pyramidal geometry with coordination by two nitrogen atoms (a pyridyl and an amide nitrogen, both from the same ligand) and two oxygen atoms (alkoxide oxygens from the two ligands of the dimer) in the basal plane and by a water molecule in the axial position. The distortion of the tetragonal pyramid is indicated by the fact that the basal donor atoms are not planar, Table 30, but deviate by as much as 0.19Å from their least-squares plane. The

nature of the distortion is indicated by the dihedral angle between the N1-Cu-N2 plane and the O1-Cu-O1′ plane, 19.8(2)°, and by the nature of the displacements from the least-squares plane; Cu, N1, and O1′ are displaced (0.16, 0.11, and 0.19Å, respectively) in the direction of the axial water molecule and N2 and O1 are displaced (both by 0.18Å) to the opposite side of the plane to give a distortion toward a trigonal-bipyramidal arrangement. As usual in the case of copper(II) complexes, the axial Cu-O distance (2.394(6)Å) is considerably longer than the Cu-O distances in the basal plane (1.951(4) and 1.946(4)Å).

An interesting feature of the molecular structure is the four-membered Cu_2O_2 ring. In CuPIPA·$2H_2O$ the dimer has twofold symmetry and the four-membered ring is bent to give a dihedral angle of 15.9(4)° between the O1-Cu-O1′ and O1-Cu′-O1′ planes (where X and X′ are related by twofold operation). The Cu-Cu distance is 2.948(3)Å, Cu-O-Cu angle is 98.3(2)° and O-Cu-O′ angle is 80.4(2)°. Bond distances and bond angles of the ligand are listed in Tables 28 and 29 and are reasonable in comparison to corresponding values in other structures. The C-H distance ranges from 0.91(6) to 1.06(6)Å, with an average value of 0.96Å, and bond angles involving hydrogens indicate reasonable geometries about the carbons.

The hydrogen bonding in the structure is relatively weak and involves the uncoordinated water molecule (O4), which serves as a proton donor to the alkoxide oxygen (O4‴-O1, 2.840(7)Å; H1O4-O4, 0.79(6)Å; H1O4‴-O1, 2.08(7)Å; O4‴-H1O4‴-O1, 168(9)° and as a proton acceptor from the coordinated water (O4-O3, 2.890(7)Å; H1O3-O3, 0.57(7)Å; H1O3-O4, 2.11(7)Å; O3-H1O3-O4; 174(6)°). Dimers are connected into chains in the

Table 27. Positional and Thermal Parameters for CuPIPA·$2H_2O$*

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	.03056(3)	.21512(9)	.18686(4)	.00146(2)	.01497(13)	.00193(2)	.00024(6)	.00090(2)	.00051(7)
N1	-.0112(3)	.2408(8)	.0576(3)	.0021(1)	.0126(14)	.0023(2)	.0004(3)	.0011(1)	-.0002(4)
N2	.1242(2)	.1518(6)	.1808(3)	.0021(2)	.0154(11)	.0029(2)	.0006(3)	.0014(2)	-.0006(4)
O1	-.0663(2)	.1870(7)	.1834(2)	.0018(1)	.0167(11)	.0020(2)	.0002(3)	.0010(1)	-.0007(3)
O2	.0245(2)	.2675(7)	-.0516(3)	.0031(2)	.0193(12)	.0029(2)	.0014(4)	.0017(1)	.0007(4)
O3	.0650(3)	.5315(7)	.2066(3)	.0034(1)	.0190(14)	.0028(2)	.0007(4)	.0014(1)	.0007(4)
O4	-.0928(3)	.8150(9)	.1567(3)	.0039(2)	.0172(11)	.0045(3)	.0002(5)	.0029(2)	.0003(5)
C1	-.1290(3)	.2741(13)	.1137(4)	.0032(2)	.0443(24)	.0034(3)	.0065(7)	.0019(2)	.0024(7)
C2A	-.1439(5)	.2294(21)	.0214(6)	.0014(3)	.0136(23)	.0018(4)	-.0011(9)	.0002(3)	-.0017(10)
C2B	-.1298(8)	.3606(28)	.0454(8)	.0023(5)	.0270(38)	.0028(6)	.0022(12)	.0006(4)	.0037(13)
C3	-.0897(2)	.2874(10)	-.0076(3)	.0017(2)	.0185(12)	.0024(2)	.0006(5)	.0006(2)	.0008(5)
C4	.0373(2)	.2381(7)	.0281(3)	.0020(1)	.0119(13)	.0023(2)	.0006(4)	.0013(1)	-.0003(4)
C5	.1165(3)	.1942(9)	.1002(3)	.0023(2)	.0128(12)	.0026(2)	.0002(4)	.0013(2)	.0002(5)
C6	.1766(3)	.1908(9)	.0836(3)	.0026(2)	.0149(13)	.0037(2)	.0006(4)	.0020(2)	.0006(5)
C7	.2464(3)	.1454(9)	.1529(4)	.0021(2)	.0198(15)	.0055(3)	.0005(4)	.0023(2)	-.0010(5)
C8	.2544(3)	.0930(9)	.2355(4)	.0022(2)	.0218(16)	.0043(4)	.0015(5)	.0017(2)	.0004(5)
C9	.1918(3)	.0978(9)	.2469(4)	.0029(2)	.0143(14)	.0035(3)	.0016(4)	.0018(2)	.0008(4)

Table 27. (Continued)

Atom	x	y	z	B
H1C1	-.172	.237	.117	4.4
H2C1	-.122	.402	.123	4.4
H1C2A	-.190	.291	-.019	3.0
H2C2A	-.149	.105	.014	3.0
H1C2B	-.106	.480	.070	3.0
H2C2B	-.181	.384	.002	3.0
H1C3	-.097(3)	.415(8)	.035(4)	3.0
H2C3	-.105(3)	.212(9)	-.068(4)	3.0
HC6	.164(3)	.229(8)	.022(4)	2.9
HC7	.286(4)	.139(9)	.142(4)	3.9
HC8	.300(3)	.058(7)	.283(4)	3.5
HC9	.194(3)	.081(7)	.302(4)	3.0
H1O3	.058(4)	.569(10)	.174(5)	3.3
H2O3	.070(4)	.602(9)	.244(5)	3.3
H1O4	-.084(4)	.907(9)	.174(5)	3.5
H2O4	-.078(4)	.775(10)	.134(5)	3.5

Atom multiplier of C2A = .52(1)
Atom multiplier of C2B = .48(1)

*The form of the anisotropic thermal ellipsoid is: $\exp[-\beta_{11}h^2-\beta_{22}k^2-\beta_{33}l^2-\beta_{12}hk-\beta_{13}hl-\beta_{23}kl]$

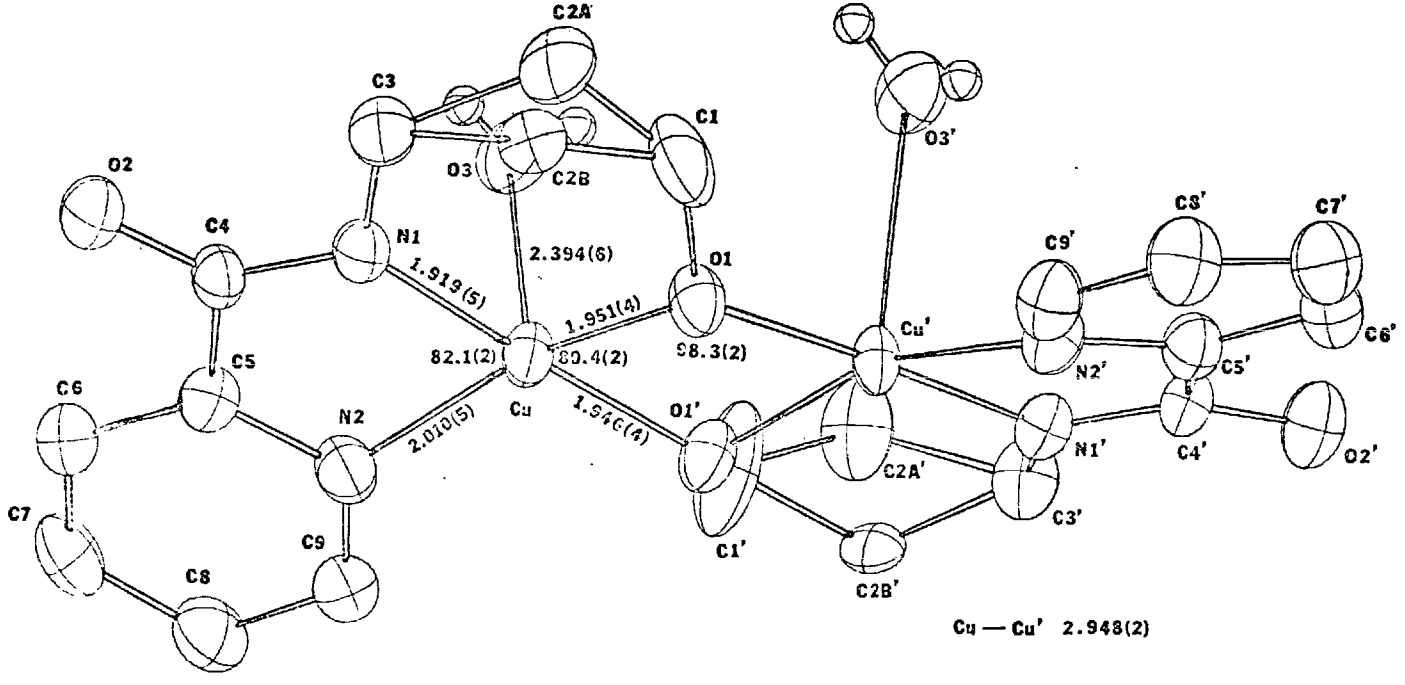


Figure 24. Structure of $[Cu(PIPA)(H_2O)]_2 \cdot 2H_2O$

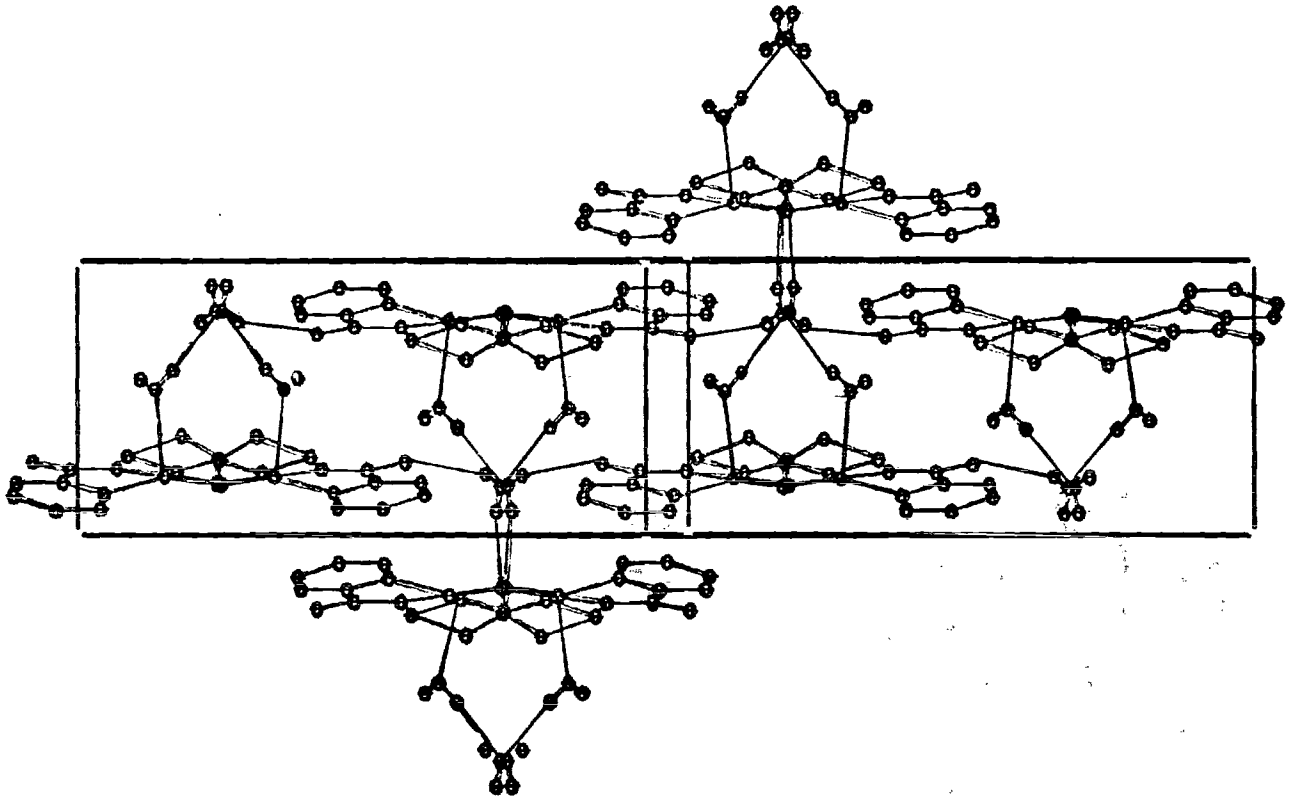


Figure 25. A Perspective View of the Crystal Packing of $[Cu(PIPA)(H_2O)]_2 \cdot 2H_2O$

Table 28. Selected Interatomic Distances for CuPIPA·$2H_2O$*

Atoms	Distance, Å	Atoms	Distance, Å
Cu-N1	1.919(5)	C2A-C3	1.471(11)
Cu-N2	2.010(5)	C2B-C3	1.571(16)
Cu-O1	1.951(4)	C4-C5	1.497(7)
Cu-O3	2.394(6)	C5-C6	1.381(7)
N1-C3	1.463(7)	C6-C7	1.361(8)
N1-C4	1.306(7)	C7-C8	1.375(8)
N2-C5	1.326(6)	C8-C9	1.378(7)
N2-C9	1.333(7)	O1-O4	2.840(7)
O1-C1	1.391(7)	O4''' -O2''	2.788(7)
O2-C4	1.254(6)	Cu-Cu'	2.948(2)
O3-O4	2.890(7)	Cu-O1'	1.946(4)
C1-C2A	1.468(11)	O4''' -O1	2.840(7)
C1-C2B	1.307(15)		

*X and X' are related by the two-fold operation. X and X'' are related by the inversion operation. X and X''' are related by a "b" translation.

Table 29. Selected Interatomic Angles for $CuPIPA \cdot 2H_2O$*

Atoms	Bond Angles, Deg.	Atoms	Bond Angles, Deg.
N1-Cu-N2	82.1(2)	Cu-O1-Cu'	98.3(2)
N1-Cu-O1	95.9(2)	Cu-O3-O4	135.2(2)
N1-Cu-O3	89.9(2)	O1-C1-C2A	114.7(6)
N2-Cu-O1'	101.3(2)	O1-C1-C2B	125.1(8)
N2-Cu-O3	90.6(2)	C1-C2A-C3	119.4(8)
O1-Cu-O1'	80.4(2)	C1-C2B-C3	123.5(13)
O1-Cu-O3	109.1(2)	C2-C3-N1	113.7(5)
O1'-Cu-O3	91.4(2)	N1-C4-O2	127.5(5)
N1-Cu-O1'	176.3(2)	N1-C4-C5	113.9(4)
N2-Cu-O1	101.3(2)	O2-C4-C5	118.6(4)
Cu-N1-C3	125.6(4)	N2-C5-C4	114.7(4)
Cu-N1-C4	116.0(3)	N2-C5-C6	122.3(5)
C3-N1-C4	117.8(4)	C4-C5-C6	122.9(4)
Cu-N2-C5	111.3(3)	C5-C6-C7	118.9(5)
Cu-N2-C9	129.6(4)	C6-C7-C8	119.3(5)
C5-N2-C9	118.5(5)	C7-C8-C9	118.6(6)
Cu-O1-C1	117.8(4)	C8-C9-N2	122.3(5)

*X and X' are related by the twofold operation.

Table 30. Equations of Least Squares Planes[a,b] and Distances (Å) of Atoms from These Planes for $CuPIPA \cdot 2H_2O$

Atom	Deviation Å	Atom	Deviation Å	Atom	Deviation Å
(a) Equation of the plane of the coordination sphere (O1, N1, N2, O1′):					
		.0645x + .9889y + .1337z = 1.7031			
Cu	.160	C1	.273	C5	-.003
N1	.107	C2A	-.201	C6	.028
N2	-.184	C2B	.800	C7	-.110
O1	-.176	C3	.248	C8	-.361
O1′	.188	C4	.109	C9	-.392
O2	.191				
(b) Equation of the plane of the five-membered chelate ring and amide oxygen (Cu, N1, N2, C4, C5, O2):					
		.1531x + .9667y + .2049z = 1.8555			
Cu	.085	N2	-.082	C4	-.006
N1	-.087	O2	.023	C5	.054
(c) Equation of the plane of pyridine ring (C5, C6, C7, C8, C9, N2)					
		.0633x + .9518y + .3002z = 1.8974			
Cu	.364	C7	.025	N2	.020
C5	-.007	C8	-.010		
C6	-.017	C9	-.013		

[a]Direction cosines of the plane refer to the orthogonal axis system a,b,c*.

[b]All atoms weighted at unity.

c direction by the O4-O2" interaction and these chains are connected into sheets in the b direction by the uncoordinated waters bridging between the O3 atoms of one chain and the O1 atoms of another chain.

CHAPTER III

DISCUSSION

Hydrogen-bonded Dinuclear Complexes in Compounds of the General Formula $MM'(Eta)_n(EtaH)_{6-n}X_2$

Hydrogen-bonded dimers of transition metal complexes were first suggested by Yoneda and Kida[5] for a series of compounds with the formula, $Co_2(Eta)_3(EtaH)_3X_3 \cdot nH_2O$. Dinuclear structures containing octahedral tris chelates with from one (corner-to-corner bonding) to three (face-to-face bonding) hydrogen bonds were considered. Recently an X-ray single crystal diffraction study confirmed that $Co_2(Eta)_3(EtaH)_3(ClO_4)_3 \cdot 1/2\ H_2O$ (Hereafter this compound will be abbreviated $Co^{III}Co^{III}EtaP$) is a face-sharing hydrogen-bonded (or face-to-face bonding) dinuclear complex. In this section, first the structure of the face-sharing hydrogen-bonded dinuclear complexes, $Co^{III}Co^{III}EtaP$, NiNiEtaP, and CoNiEtaI (where NiNiEtaP and CoNiEtaI represent $Ni_2(Eta)_2(EtaH)_4(ClO_4)_2$ and $CoNi(Eta)_3(EtaH)_3I_2$, respectively) and the structure of Co-trimer (where Co-trimer represents $Co_3(Eta)_6(OAc)_2$) will be compared. Then the magnetic properties of NiNiEtaP will be discussed. Concluding this section will be a description of various mixed-metal dinuclear complexes with 2-aminoethanol and with the formula: $MM'(Eta)_n(EtaH)_{6-n}(ClO_4)_2$.

The cation of the NiNiEtaP structure (Figure 12) studied in this work is closely related to the cations present in $Co^{III}Co^{III}EtaP$,[50] CoNiEtaI[9] (Figure 4), and Co-trimer[8] (Figure 3). In $Co^{III}Co^{III}EtaP$,

three hydrogen bonds between oxygen faces link the two tris-chelate metal complexes into a dinuclear unit which has a twofold axis perpendicular to the metal-metal axis. All hydrogens were located and one of the hydrogens which participates in the hydrogen-bonding is on the twofold axis. In the isomorphous structures of CoNiEtaI and NiNiEtaP, similar dinuclear units occupy sites of threefold inversion symmetry. Although both metal atoms and all ligands of the dinuclear unit should be symmetry related, the difference between Co-O and Ni-O bond distances in CoNiEtaI and the presence of only two hydrogen bonds instead of three in NiNiEtaP dictate that two sets of disordered ligand positions must be located for each of these structures. For CoNiEtaI, the two sets of ligand positions, each with an occupancy factor of 0.5 were used in refining the structure. In NiNiEtaP, the occupancy factors refined to the values of 0.69 and 0.31 rather than 1/2. These values indicate four ligands of one type and two of another type for each dimeric unit and the values are consistent with the existence of two short hydrogen bonded oxygen-oxygen distances between the disordered ligands (2.24Å). The structure of the Co-trimer consists of a linear arrangement of three cobalts; there is octahedral coordination about the terminal cobalt(III) atoms and trigonal prismatic coordination about the central cobalt(II) atom. Although the Co-trimer does not have intermolecular hydrogen-bonding, the structure is similar to the structure of the intramolecular hydrogen bonded cobalt dimer, $Co^{III}Co^{III}$EtaP. This similarity may be demonstrated by removing the central cobalt of the trimer and placing three protons between the three associated pair of oxygen atoms of the 2-aminoethanol ligands on the remaining two cobalt atoms.

Table 31 shows the crystallographic data and bond distances of these compounds. The metal-metal distances in NiNiEtaP (4.582(2)Å), CoNiEtaI (4.650(3)Å), and $Co^{III}Co^{III}$EtaP (4.538(4)Å) are quite similar. The Co(III)-oxygen distances (from 1.88 to 1.98Å) in $Co^{III}Co^{III}$EtaP and Co-trimer and the Ni(II)-oxygen distances (2.07 and 2.10Å) in NiNiEtaP reveal that the metal-oxygen distances of 1.92(2) and 2.09(2)Å in CoNiEtaI are Co(III)-oxygen and Ni(II)-oxygen distances, respectively. The Co(III)-nitrogen distances (from 1.88 to 2.02Å) in $Co^{III}Co^{III}$EtaP and Co-trimer and Ni(II)-nitrogen distances (2.08 and 2.05Å) in NiNiEtaP reveal that the metal-nitrogen distances of 2.07(3) and 2.12(3)Å in CoNiEtaI are Co(III)-nitrogen and Ni(II)-nitrogen distances. The cobalt(III)-nitrogen distances are slightly longer than those in $Co^{III}Co^{III}$EtaP and Co-trimer. The oxygen-oxygen distances of the hydrogen bonds in $Co^{III}Co^{III}$EtaP are 2.396(10) and 2.442(7)Å and hydrogens were placed midway between the oxygen atoms. It is not known whether these positions are truly refined positions or the average of two disordered positions related by the twofold axis. In NiNiEtaP, the two very short oxygen-oxygen distances of 2.24(3)Å exist due to the disorder of the ligand. Although this short distance was calculated from the positions of disordered oxygens, this value may contain cumulative errors due to the refinement of disordered atoms. For example, the C-N distance of 1.58(3)Å and the C-O distance of 1.34(5)Å in ligand B are slightly longer and shorter than typical C-N and C-O bonds in similar complexes. The calculated distance between the two hydrogen-bonded oxygen atoms in CoNiEtaI is 2.51Å.

Because a tris-chelated complex is optically active, there are

Table 31. Crystallographic Data and Bond Distances for NiNiEtaP, CoNiEtaI, $Co^{III}Co^{III}$EtaP and Co-trimer

	NiNiEtaP	CoNiEtaI	$Co^{III}Co^{III}$EtaP	Co-trimer
Space group	Pa3	Pa3	P2/c	C2/m
Unit cell	a = 13.85(1)Å	a = 13.60Å	a = 12.13	a = 14.98(3)Å
			b = 8.78	b = 8.61(2)Å
			c = 16.50	c = 11.28(3)Å
			β = 121.39	β = 116.7(1)°
Z	2	2	2	2
Calc'd density $g \cdot cm^{-3}$	1.67	1.93	1.75	1.68
Obs. density $g \cdot cm^{-3}$	1.65	1.94	1.74	1.66
M-M	4.582(2)	4.650(3)	4.538(1)	5.194(10)
M-O1	A 2.07(1)	A 1.92(2)	1.894(5)	1.975(5)
M-O2	B 2.10(3)	B 2.09(2)	1.907(5)	1.885(7)
M-O3			1.907(5)	1.93(2)
M-N1	A 2.08(1)	A 2.07(3)	1.940(7)	1.88(2)
M-N2	B 2.05(3)	B 2.13(2)	1.940(7)	1.99(2)
M-N3			1.944(6)	2.02(3)
O-O'	2.24(3)	2.51(3)	2.396(10)	2.79(1)
			2.442(7)	2.80(2)
			2.442(7)	2.80(2)

three possible combinations of optically active monomers for a dimer composed of two tris-chelated or for a linear trimer composed of two tris-chelated unit surrounging a central metal. These combinations are a meso complex, involving a Δ-Λ pair, and two optically active complexes, involving Δ-Δ and Λ-Λ pairs. Actually the cations hexakis(2-aminoethanethiolo)tricobalt(III), $Co_3(Teta)_6^{3+}$, and hexakis(2-aminoethanethiolo)-dicobalt(III)zinc(II), $Co_2Zn(Teta)_6^{2+}$, have been separated into meso (Δ-Λ isomers for the terminal cobalts) and optically active (Δ-Δ isomers and Λ-Λ isomers for the terminal cobalts) forms using a cation-exchange cellulose column[51] and silver antimony d-tartrate.[52] In addition the electronic and circular dichroism spectra were reported for the optical isomers. Since only the terminal cobalt(III) ions contribute to the visible CD spectrum of the heterometallic complex ion, this spectrum was substracted from that for the tricobalt(III) complex to obtain the CD spectrum of the central cobalt. Opposite configurations about the central and terminal cobalt ions were assigned from the CD spectra. Although it was assumed that the central metals have octahedral geometries for both cations, the same conclusion for absolute configurations may be drawn for a trigonal prismatic arrangement of the central metal. However, the coordination of the central metal atom is not known for any isomer of these complexes.

$Co^{III}Co^{III}$EtaP with a trigonal prismatic arrangement of oxygen atoms coordinated to cobalt contains Δ-Δ isomers (and Λ-Λ isomers) with twofold symmetry. In order to explore the possibility of the existence of other isomers, steric hindrances of hydrogens of α-carbons were

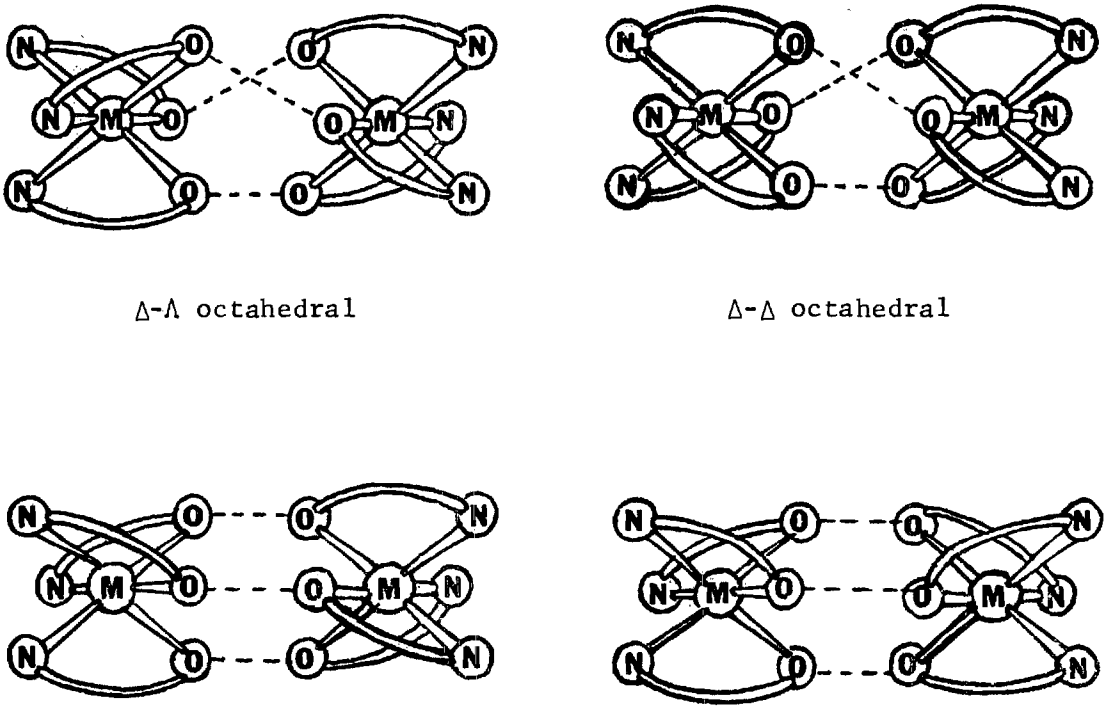


Figure 26. Various Isomers for Hydrogen-Bonded Dinuclear Complexes of Tris-2-aminoethanol Metal Species

considered.[50] To compare the hydrogen-hydrogen distances of the hydrogens on the α-carbons for a Δ-Δ isomer with twofold symmetry (the Δ-Δ trigonal prismatic isomer shown in Figure 26) with comparable distances in Δ-Δ octahedral, Δ-Λ trigonal prismatic, and Δ-Λ octahedral isomers (Figure 26), pseudo-symmetry operations were carried out using crystallographic data, such as a, b, c, β and x, y, z coordinates of cobalt atoms to transform the positions of hydrogen atoms of $Co^{III}Co^{III}$EtaP. The Δ-Δ octahedral

isomer corresponds to two Δ-monomers arranged such that on each monomer the octahedral faces containing three coordinated oxygen atoms are parallel and centered on the cobalt-cobalt axis with the six oxygen atoms in a staggered conformation. In the Δ-Δ octahedral isomer the atoms of one monomer are related to the atom in the other monomer by a 180° rotation in one direction and a 60° rotation in a direction which is perpendicular to the first rotation and coincident with the metal-metal axis. The Δ-Λ octahedral isomer corresponds to one Δ monomer and one Λ monomer arranged such that on each monomer the octahedral faces containing three coordinated oxygen atoms are parallel and centered on the cobalt-cobalt axis with the six oxygen atoms in a staggered conformation. In the Δ-Λ octahedral isomer the atoms of one monomer are related to the atoms of the other monomer by a center of inversion. The Δ-Λ trigonal prismatic isomer is related to the Δ-Λ octahedral isomer by a rotation of one monomer about the metal-metal axis to form an eclipsed conformation. In the Δ-Λ trigonal prismatic isomer the atoms of one monomer related to the atoms of the other monomer by inversion and a rotation of 60° about an axis coincident with the metal-metal axis. The Δ-Δ trigonal prismatic isomer corresponds to the Δ-Δ octahedral isomer with one monomer unit rotated to make the six oxygen atoms eclipsed. In the Δ-Δ trigonal prismatic isomer the atoms in one monomer are related to the atoms in the other monomer by a 180° rotation perpendicular to the metal-metal axis. Calculated distances for the Δ-Λ trigonal prismatic isomer and Δ-Δ octahedral isomer indicate that there exist several hydrogen-hydrogen distances less than twice the Van der Waals radius of hydrogen (2.2Å). On the other hand, all hydrogen-hydrogen distances for the Δ-Δ

trigonal prismatic isomer and the Δ-Λ octahedral isomer are longer than 2.6Å. Therefore the possibility of the existence of a Δ-Λ trigonal prismatic isomer and a Δ-Δ octahedral isomer may be excluded. Although the Δ-Λ octahedral isomer of $Co^{III}Co^{III}$EtaP has not been isolated, NiNiEtaP and CoNiEtaI are Δ-Λ octahedral isomers. Due to the disorder of ligands, the hydrogen distance calculations to determine the existence of isomers could not be carried out.

The magnetic moment of NiNiEtaP in Table 5 indicates very weak antiferromagnetic coupling. On changing temperature from 298 to 93 °K the magnetic moment of NiNiEtaP decreases by only 0.12BM per gram atom of nickel. Although this compound has short hydrogen bonds (2.24Å), the magnitude of the magnetic coupling is inconsistent with the magnetic coupling of similar strong intramolecularly hydrogen bonded complexes.

Although compounds of the general formula $MM'(Eta)_n(EtaH)_{6-n}(ClO_4)_2$ (where M = Ni and M′ = Fe, Mn, Zn, Cr, and Co; and where M = Co and M′ = Fe, Mn, Mg, Zn, and Co) were prepared under aerobic conditions, the two metal atoms were not present in a 1:1 ratio and in the cobalt compounds the cobalt was a mixture of cobalt(II) and cobalt(III). However, $Co(II)_2(Eta)_2(EtaH)_4(ClO_4)_2$ was prepared under a nitrogen atmosphere, and $Co(III)_2(Eta)_3(EtaH)_3(ClO_4)_3$, instead of $Co(III)_2(Eta)_4(EtaH)_2(ClO_4)_2$, was isolated in an oxygen atmosphere. These mixed metal materials are essentially insoluble in non-polar solvents, and are decomposed in water and alcohols; hence the usual spectroscopic studies of solutions and chromatographic isolation are inappropriate. For M = Ni and M′ = Fe, Mn, and Zn, analytical data indicate a greater nickel content than a 1:1

metal ratio requires. For M = Co(II,III) and M′ = Fe, Mn, and Mg, analytical data show a greater cobalt content than a 1:1 metal ratio requires. These results may indicate that the M-M and M-M′ species are the major species in solution. This is reasonable if it is assumed that all of the material in solution initially is present as the M-M dinuclear species and addition of M′ preferentially forms the M-M′ species. The fact that the pure M′-M′ compounds could not be isolated under the same conditions used for the M-M compounds may indicate that the M′-M′ compounds are more soluble and are, thus, not precipitated with the M-M′ compound. Because of the method of preparation of $NiCr(Eta)_3(EtaH)_3(ClO_4)_2$, more chromium content can be expected, and this is confirmed by analytical results. Under atmospheric conditions $Co(II,III)Ni(Eta)_n(EtaH)_{6-n}(ClO_4)_2$ was prepared by two different methods. The compound prepared by the addition of a solution of Co^{2+} to a solution of $Ni_2(Eta)_2(EtaH)_4(ClO_4)_2$ contained more nickel. The compound prepared by the addition of a solution of Ni^{2+} into a solution of $Co(II,III)_2(Eta)_n(EtaH)_{6-n}(ClO_4)_2$ contained more cobalt.

At this point the exact nature of the M-M′ compounds may be questioned. There is a distinct possibility that these compounds are solid solutions with an accidentally equimolar quantity of M and M′. It is impossible to distinguish between a homogeneous structure with M-M′ dinuclear cations and a solid solution of M-M and M-M′ cations by X-ray diffraction. It is also difficult to distinguish these by the comparison of magnetic moments between compounds like CoNiEtaI and NiNiEtaP, due to the very weak magnetic coupling of NiNiEtaP. A homogeneous structure with cobalt-nickel dinuclear cations might be considered, since

$Ni_2(Eta)_2(EtaH)_4^{2+}$ and $Co(III)_2(Eta)_3(EtaH)_3^{3+}$ were isolated, but $Co(III)_2(Eta)_4(EtaH)_2^{2+}$ was not isolated. For an equimolar mixture of $Co(III)_2(Eta)_3(EtaH)_3^{3+}$ and $Ni_2(Eta)_2(EtaH)_4^{2+}$ there cannot be an integral number of iodide anions. Elemental analysis dictates that the formula for the cobalt-nickel complex is $CoNi(Eta)_3(EtaH)_3I_2$.

Hydrogen-bonded Dinuclear Complexes in the Compounds of the General Formula $Cu(L)(LH)X \cdot nH_2O$

Unusual magnetic properties indicative of antiferromagnetic behavior have been noted for a number of polynuclear copper compounds with Cu_2X_2 four-membered Cu_2X_2 rings (where X = O , Cl).[2,53,54] In all of the compounds for which structural information is available, the metal-metal distance is sufficiently large to make direct magnetic interaction unlikely. In fact, there is no correlation between the copper-copper distance and the magnitude of the coupling constant. It is now generally considered that the coupling in these compounds occurs by superexchange through the bridging groups, but the pathway or mechanism of exchange is still under consideration.

The molecular orbital approach was used to explain the magnetic coupling through a sigma and/or a pi pathway.[2,55,56] In square planar copper(II) dimers the unpaired electron on each copper would be in the d_{xy} orbital. Assuming C_{2h} symmetry, these two half-filled d_{xy} orbitals would be combined into linear combinations which transform with A_g and B_u representations and these would interact with s and p orbitals on the bridging atoms. Considering only the p_x and p_y orbitals on the bridging groups, the pair of p_x orbitals and the pair of p_y orbitals,

although of different symmetries, would have identical overlaps with the pair of d_{xy} orbitals for a bridge angle (Cu-X-Cu) of 90°. Thus the two different symmetry combinations would give molecular orbitals of equal energies, but distortion of the bridge angle away from 90° would destroy the accidental degeneracy. Therefore, antiferromagnetic behavior would be expected. When the s orbitals of bridging atoms are considered, these atomic orbitals would mix into the B_u molecular orbitals, and the overlap at 90° would not be the same for A_g and B_u combinations. The accidental degeneracy would be expected to occur at some angle other than 90°, and ferromagnetic behavior would be expected at this angle. In agreement with these predictions, interesting linear relationships between the Cu-X-Cu (where X = O and Cl) angle and magnetic coupling were found for hydroxy-bridged[52] and chloro-bridged[53] copper(II) complexes.

In order to understand the mechanism or pathway of magnetic coupling in hydrogen-bonded dimers, several hydrogen-bonded copper complexes of 2-aminoethanol and substituted 2-aminoethanols were prepared and compared as to oxygen-oxygen distances, the geometry of the hydrogen-bonded ring, and the magnitude of the magnetic interaction. Detailed magnetic susceptibilities and magnetic moments per gram atom of copper of these compounds at various temperatures are listed in Tables 6, 32, 33, and 34.

The nitrogen-oxygen hydrogen-bonded trinuclear copper complex with ℓ-ephedrine, $[Cu(\ell\text{-Eph})_2]_3 \cdot 2C_6H_6$, exhibited no magnetic coupling over the temperature range studied. This behavior may be related to the weak hydrogen bonds (2.87Å).

Table 32. Experimental Magnetic Susceptibilities of a Dimer (2χ) and Calculated Values Using the Bleany and Bowers Equation for Cu(ℓ-Eph): $2J = -49\ cm^{-1}$, $g = 2.25$, and $N\alpha = 62 \times 10^{-6}$cgsu

T(°K)	obs. $2\chi(\times 10^3$cgsu)	calc'd $2\chi(\times 10^3$cgsu)
298	3.085	3.049
295	3.107	3.077
283	3.189	3.195
273	3.298	3.301
263	3.410	3.414
253	3.534	3.536
243	3.617	3.666
233	3.812	3.806
223	3.948	3.958
213	4.116	4.122
203	4.294	4.300
193	4.491	4.494
183	4.705	4.705
173	4.932	4.938
163	5.190	5.194
153	5.466	5.477
143	5.766	5.791
133	6.230	6.141
123	6.575	6.533
113	6.923	6.972
103	7.478	7.467
93	8.009	8.022

Table 33. Experimental Magnetic Susceptibilities of a Dimer (2χ) and Calculated Values Using the Bleany and Bowers Equation for for CuEta: $2J = -56\ cm^{-1}$, $g = 2.11$, and $N\alpha = 59 \times 10^{-6}$cgsu

T(°K)	obs. $2\chi(\times 10^3$cgsu)	calc'd $2\chi(\times 10^3$cgsu)
298	2.628	2.663
293	2.710	2.704
283	2.812	2.789
273	2.884	2.880
263	2.968	2.977
253	3.078	3.081
243	3.184	3.192
233	3.332	3.312
223	3.458	3.441
213	3.550	3.580
203	3.738	3.731
193	3.878	3.894
183	4.116	4.073
173	4.264	4.267
163	4.468	4.481
153	4.736	4.715
143	4.970	4.974
133	5.250	5.260
123	5.548	5.576
113	5.992	5.926
103	6.234	6.313
93	6.746	6.736
91	6.848	6.825

Table 34. Experimental Magnetic Susceptibilities of a Dimer (2χ) and Calculated Values Using the Bleany and Bowers Equation for CuMep: $2J = -70\ cm^{-1}$, $g = 2.18$, and $N\alpha = 99 \times 10^{-6}$cgsu

T(°K)	obs. $2\chi(\times 10^3$cgsu)	calc'd $2\chi(\times 10^3$cgsu)
298	2.831	2.814
293	2.863	2.856
283	2.928	2.942
273	3.049	3.034
263	3.129	3.132
253	3.258	3.236
243	3.350	3.347
233	3.438	3.467
223	3.564	3.595
213	3.711	3.732
203	3.872	3.800
193	4.038	4.040
183	4.222	4.213
173	4.384	4.400
163	4.652	4.604
153	4.844	4.824
143	5.090	5.064
133	5.317	5.324
123	5.569	5.605
113	5.860	5.906
103	6.290	6.224
93	6.531	6.550

On the other hand, oxygen-oxygen hydrogen-bonded dinuclear complexes such as CuEta, CuMep, and Cu(ℓ-Eph)(where CuEta, CuMep, and Cu(ℓ-Eph) represent $[Cu(Eta)(EtaH)]_2(NO_3)_2$, $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$, and $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$, respectively) exhibited weak antiferromagnetic coupling. 2J, g, and Nα values of these hydrogen-bonded compounds were evaluated by least square fitting methods using the Bleany and Bowers equation. The results are shown in Tables 32, 33, and 34.

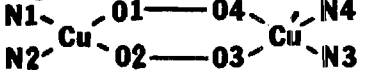
Although chelated copper complexes of CuEta, CuMep, Cu(ℓ-Eph) and CuDiimH[19,20] (where CuDiimH represents $[CuDiimH]_2$) are associated into hydrogen-bonded dinuclear units, there exist only a few differences in their structural features. The two coordination planes of CuEta, CuMep, and CuDiimH are parallel as a result of a center of inversion. The separations of the two parallel planes of these complexes are listed in Table 35. In Cu(ℓ-Eph), there is no inversion center and the two coordination planes around copper are not parallel, due to the steric hindrance of the phenyl groups. The dihedral angle of the two coordination planes is about 40°. In order to compare the structural properties of these hydrogen-bonded complexes, selected bond distances and bond angles are listed in Table 35. In Table 35 the four copper complexes are listed with increasing antiferromagnetic coupling constants (2J) from left to right.

From Table 35, it can be readily seen that although the strongest coupling occurs for the compound (CuDiimH) with the shortest oxygen-oxygen distance, there is no simple correlation between the magnitude of the antiferromagnetic coupling (2J) and the oxygen-oxygen distance of hydrogen bonds. There is also no correlation between the 2J values and

Table 35. Some Magnetic and Structural Properties for Cu(ℓ-Eph), CuEta, CuMep, and CuDiimH[a]

		Cu(ℓ-Eph)	CuEta		CuMep	CuDiimH	
			A	B		A	B
$2J\ cm^{-1}$		-49	-56		-70	-94	
g		2.25	2.11		2.18	2.04	
$N\alpha \times 10^{6}$ cgsu		62	59		99	118	
Cu-Cu′	Å	4.850	4.940	4.942	4.934	4.989	4.987
O1-O4	Å	2.39	2.452	2.434	2.516	2.33	2.31
O2-O3	Å	2.43	2.452	2.434	2.516	2.33	2.31
avg. Cu-O	Å	1.91	1.958	1.957	1.955	1.947	1.947
avg. Cu-N	Å	2.01	1.990	1.988	2.004	1.898	1.912
separation of two planes	Å	--	1.414	1.264	1.821	0.500	0.224
distance of Cu from its coordination plane	Å	.05 and .03	.001		.004	.169	
O1-Cu-O2	deg.	89.8	91.4	91.1	93.9	93.1	92.8
O4-Cu′-O3	deg.	89.7	91.4	91.1	93.9	93.1	92.8
Cu-O1-O4	deg.	120.7	124.3	123.5	130.6	133.3	134.6
O1-O4-Cu′	deg.	118.1	125.1	126.8	117.2	131.6	132.1
Cu-O2-O3	deg.	118.8	125.1	126.8	117.2	131.6	132.1
O2-O3-Cu′	deg.	121.9	124.3	123.5	130.6	133.3	134.6

[a]Numbering scheme of atoms is shown below.



Xn and X(n+2) (where X is oxygen or nitrogen atom and n is 1 or 2) are related by an inversion center for CuEta, CuMep, and CuDiimH.

the copper-copper distances or the separation of the coordination planes of associated monomeric units. There appears to be some correlation between the O1-Cu-O2 angle and the 2J values, but the significance of this correlation is not clear. It is possible that several of these geometrical factors have an effect on the magnitude of the magnetic coupling.

Since charge-transfer bands indicate degree of delocalization of an electron from metal to the ligand orbital or vice versa, the energies of charge-transfer bands of absorption spectra of these compounds might be expected to show some correlation with the magnetic coupling. But charge-transfer bands in the range of 300-700nm were not observed in the spectra (shown in Figure 11) measured by the opal glass method. Since these compounds are decomposed in water and alcohols, solution spectra could not be obtained. From the spectra of the solids, energies of the d-d transitions of these compounds could be obtained and are shown below.

Cu(ℓ-Eph)	λ_{max} = 548nm,	2J = -49 cm^{-1}
CuEta	λ_{max} = 587nm,	2J = -56 cm^{-1}
CuMep	λ_{max} = 625nm,	2J = -70 cm^{-1}

Although there appears to be a correlation between the magnitude of antiferromagnetic coupling and the d-d transition energy, the basis of such a correlation is not apparent.

Although the copper complex of N,N'-dimethyl-2-aminoethanol (CuDme) has the same empirical formula as the copper complex of 2-aminoethanol and other substituted 2-aminoethanols, it showed strong antiferromagnetic

behavior. Preliminary crystallographic results indicate a trinuclear structure, and the different magnetic behavior might be the result of a different type of structure.

A Tetramer CoDeta, A Type of Titanium Alkoxide Structures

The compound, $[Co(II)Co(III)(Deta)_2(DetaH_2)]_2(ClO_4)_2$ (Hereafter this will be abbreviated as CoDeta) was prepared by a slight modification of the published method.[25] According to this paper, this compound contained one water molecule per two cobalt atoms. The density measurement and final difference map confirmed that CoDeta did not contain any water molecules.

The arrangement of metal atoms and bridging alkoxide oxygen atoms of CoDeta is similar to that of titanium alkoxides. The interface Co2 atoms have a severely distorted octahedral geometry with one amine nitrogen atom, two μ_3-alkoxide oxygen atoms, two μ-alkoxide oxygen atoms, and one alcohol oxygen atom. The Co2-coordinating atom distances are Co-N of 2.241(4)Å, two Co-O's of 2.161(3) and 2.225(3)Å, two Co-O's of 2.053(3) and 2.045(3)Å, and a Co-O of 2.103(4)Å, respectively. The outer-corner Co atom, Co1, has octahedral geometry with two amine nitrogen atoms, one μ_3-alkoxide oxygen atom, two μ-alkoxide oxygen atoms, and one alkoxide oxygen atom. The Co1-coordinating atom distances are Co-N's of 1.968(4) and 1.957(4)Å, a Co-O of 1.904(3)Å, two Co-O's of 1.893(3) and 1.888(3)Å, and a Co-O of 1.940(3)Å. All of these bond distances are shorter than the corresponding bond distances for Co2. The Co-N bond distances in $Co(NH_3)_6^{3+}$ and $Co(NH_3)_6^{2+}$ were reported as 1.96(2) and 2.11(1)Å, respectively.[57] A cubane-type complex containing both cobalt(II) and cobalt(III)

has been prepared by oxidation of a mixture of cobalt(II) acetate, 2,4-pentanedione, and potassium hydroxide in methanol with hydrogen peroxide.[58] The structure of this compound, di-μ-acetato-tetrakis-[μ_3-methoxo-2,4-pentanedionatocobalt(II,III)] (Hereafter this compound will be abbreviated as Co-cubane) is shown in Figure 27. All of the Co-O distances for the upper two cobalts in Figure 27 (1.83-1.94Å) were shorter than those of the lower two cobalt (1.99-2.16Å). Therefore, it was assumed that the upper two cobalt ions are trivalent and the lower two divalent. From the Co-N distances in hexammine cobalt complexes and the Co-O distances in this Co-cubane, Co1 and Co2 in CoDeta can be assigned as cobalt(III) and cobalt(II), respectively.

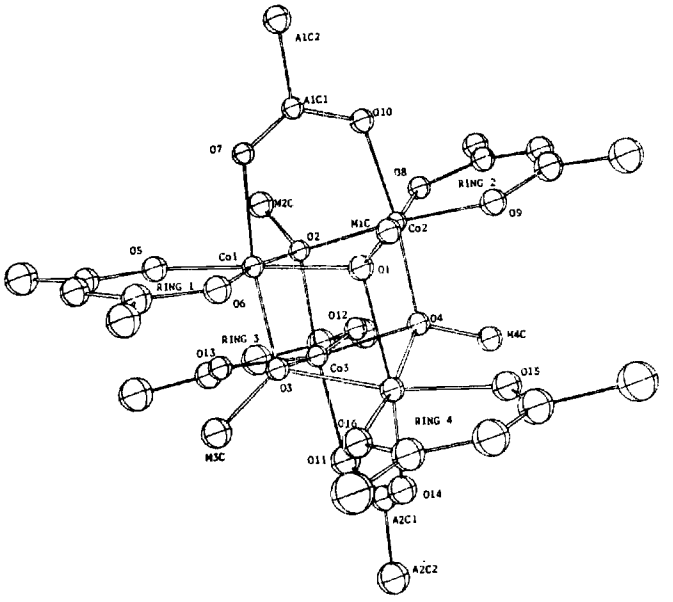


Figure 27. A Perspective Drawing of the Molecular Structure of $[Co_4(CH_3O)_4(C_5H_7O_2)_4(C_2H_3O_2)_2]$

The neutral 2,2′-dihydroxydiethylamine ligand coordinated to Co2 has one uncoordinated alcohol oxygen atom. This alcohol group is associated to one of the μ-alkoxide oxygens, O12", by weak hydrogen bond. (Where X and X" are related by twofold screw operation.) Although the tetramers are connected into chains by the hydrogen bonds, it is not known whether this hydrogen bonding pathway contributes to the magnetic coupling.

Assuming that the cobalt(III) ions are diamagnetic, the room temperature magnetic moment per gram atom of cobalt(II), 5.19BM, is in the normal range for octahedral coordination. The moment is, however, temperature dependent, decreasing to a value of 5.07BM per gram atom of cobalt(II) at 93°K; the cobalt(II) ions, thus, show weak antiferromagnetic coupling.

Co-cubane shows slightly stronger magnetic coupling (4.98BM at room temperature and 4.62BM at liquid N_2 temperature) than CoDeta. Assuming that the magnetic coupling only occurs between cobalt(II) ions, both compounds contain a Co_2O_2 four membered ring—a planar ring for CoDeta and a bent ring (dihedral angle between two O-Co-O plane is 36.3°) for Co-cubane. Additional bridging by the acetate ion in the Co-cubane may provide an additional coupling pathway and may contribute to stronger antiferromagnetic coupling.

A Dimeric Species with a Bent Four-membered Cu_2O_2 Ring, CuPIPA·$2H_2O$

The measurements of the magnetic moment of CuPIPA·$2H_2O$ approximately agree with that reported by Inoue, et al.[33] The values at 298, 195, and 77°K (Inoue's values in parentheses) are 1.48 (1.45), 1.38 (1.31), and

0.70 (0.70) BM per gram atom of copper, respectively. The moment at room temperature is considerably below the spin only value for copper(II) but is well above the moment found for the strongly coupled planar dimers (μ_{eff} = ca. 0.5BM).[2]

The previous workers[33] found that the magnetic susceptibility of CuPIPA·$2H_2O$ could not be fit to the Bleany and Bowers equation for a dinuclear copper complex. The magnetic susceptibilities for polymeric rings of various sizes were calculated numerically by the Bonner and Fisher Equation.[59] The theoretical curves are shown in Figure 28. The

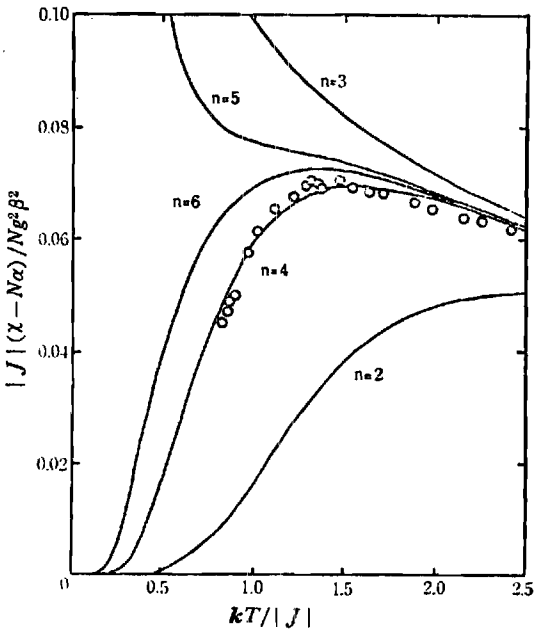
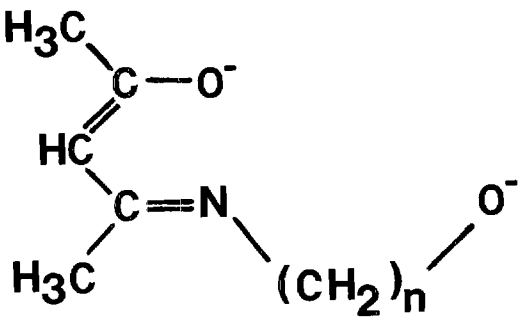


Figure 28. Observed Magnetic Susceptibility of CuPIPA·$2H_2O$ and Theoretical Curves Calculated by the Bonner and Fisher Equation

observed susceptibility for this compound apparently fits the curve for a ring composed of an even number of spins, and in particular that for a four-membered ring. 2J and g values were estimated as -128 cm^{-1} and 2.08, respectively. However, the observed values did not agree perfectly with the theoretical curve in the entire range investigated.

The X-ray structural analysis of $CuPIPA \cdot 2H_2O$ has revealed dimeric units of $[CuPIPA(H_2O)]_2$ with waters of crystallization linked by weak hydrogen bonding into an infinite planar network. The coordination of the copper(II) atom is a slightly distorted tetragonal pyramid with the weakly coordinated water molecule (Cu-O, 2.394(6)Å) in the axial position. An interesting feature of the molecular structure is the geometry of the four-membered Cu_2O_2 ring. Unlike oxygen-bridged copper(II) dimers which crystallize with the dimer on an inversion center[2,35,60,61] and thus have a planar Cu_2O_2 ring, in $[CuPIPA(H_2O)]_2 \cdot 2H_2O$ the dimer has twofold symmetry and the four-membered ring is bent to give a dihedral angle of 15.9(4)° for the O1-Cu-O1′ and the O1-Cu′-O1′ planes. (X and X′ are related by twofold operation.) The extent of bending is slightly greater than that observed in the tetrameric copper complex with the tridentate ligand I (Figure 29), $[Cu(EIA)]_4$,[60] of which the structure is shown in Figure 30.

In $[Cu(EIA)]_4$ the dihedral angle of ca. 12° is considerably less than that of the corresponding nickel dimer,[62] $[Ni(EIA)]_2$, in which the dihedral angle is 39°. The effect of this bending on the copper-copper distance, the Cu-O-Cu angle, and the O-Cu-O angle can be seen by comparing these parameters for the bent rings in $[CuPIPA(H_2O)]_2$ and in $[Cu(EIA)]_4$ with those for the planar ring in $[Cu(PIA)]_2$[60] (where PIA



ligand I, EIA, n = 2

ligand II, PIA, n = 3

Figure 29. Imines of Aminoalcohols and 2,4-Pentanedione, EIA and PIA

represents the ligand II). The structure of $[Cu(PIA)]_2$ is shown in Figure 31. The Cu-Cu distance is 2.948(3)Å in $[CuPIPA(H_2O]_2$, 3.006(8)Å in $[Cu(EIA)]_4$, and 3.026(6)Å in $[Cu(PIA)]_2$; the Cu-O-Cu angles for the same three compounds are 98.3(2), 97.8(8), and 106.4(6)° and the corresponding O-Cu-O angles are 80.4(2), 81.4(8), and 73.6(6)°. The bent ring compounds thus show decreased copper-copper distances, decreased angles at oxygen, and increased angles at copper with respect to the planar compound.

The magnetic moments of $CuPIPA \cdot 2H_2O$ at different temperatures are indicative of antiferromagnetic coupling that is weak in comparison to the coupling observed for planar, oxygen-bridged dimers. The principal antiferromagnetic coupling is undoubtedly related to superexchange within the four-membered Cu_2O_2 ring. The nonplanar nature of the ring should

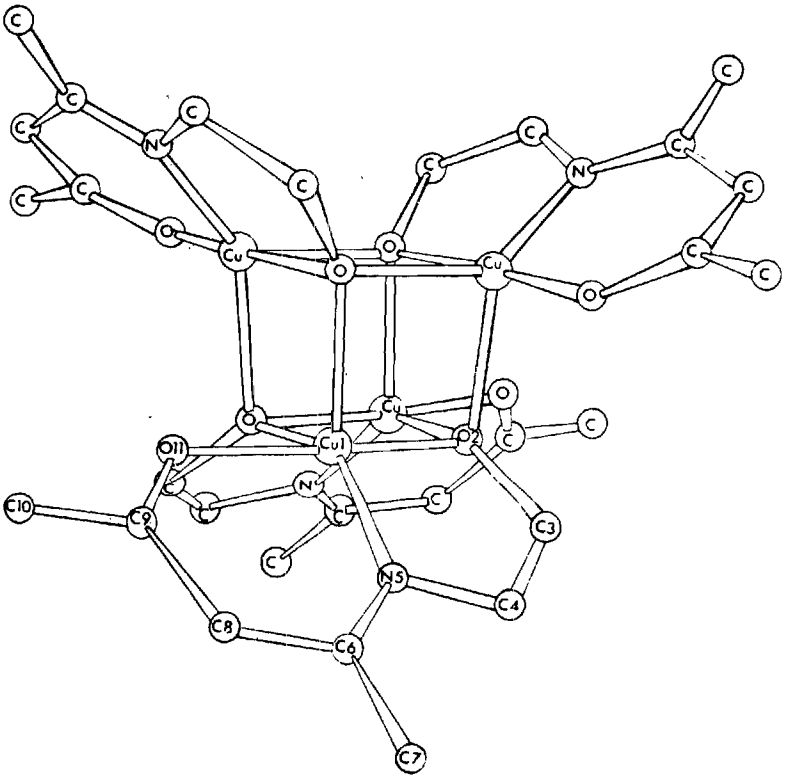


Figure 30. The Structure of a Tetrameric, Cubane-type Complex of Copper(II) and the Imine of 2,4-Pentanedione and 2-Aminoethanol

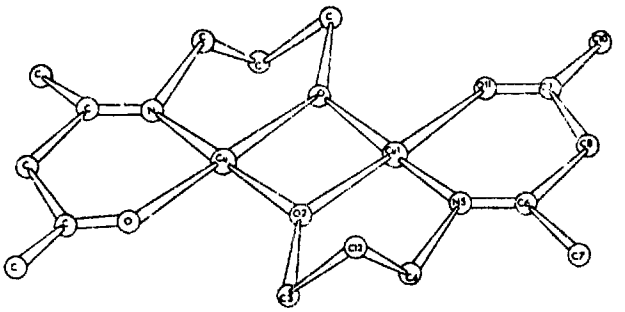


Figure 31. The Molecular Structure of Cu(PIA)

diminish markedly the importance of a potential pi pathway for superexchange. This structure, thus, provides additional evidence for superexchange through a sigma pathway. The weak coupling in the present compound and the small Cu-O-Cu angle are also in line with geometric correlation for hydroxy-bridged[53] complexes and chloro-bridged[54] complexes.

The variation of the magnetic susceptibility with temperature could not be fit to the Bleany-Bowers equation for dimers. The discrepancy probably results from interactions between clusters, possibly through the hydrogen-bonded network.

CHAPTER IV

CONCLUSIONS

Because of the possibility of widely varied structures with interesting magnetic properties, several transition metal polynuclear complexes with aminoalcohols and iminoalcohols as ligands were prepared and studied. X-ray single crystal diffraction studies revealed complexes joined into dimers by face-sharing or edge-sharing hydrogen-bonding, and oxygen-bridged oligomers with hydrogen-bonded networks or chains.

One hydrogen-bonded dinuclear complex, NiNiEtaP, is isomorphous with CoNiEtaI which was studied previously. The magnetic moment of NiNiEtaP indicates very weak antiferromagnetic coupling. It is surprising that various solids with the formula, $MM'(Eta)_n(Eta)_{6-n}(ClO_4)_2$, were separated and were found to belong to space group Pa3 with almost the same unit cell parameters. Since M and M′ can be divalent or trivalent metal ions, deprotonation of the alcoholic OH of 2-aminoethanol is extremely dependent on the conditions of preparation.

Edge-sharing hydrogen-bonded dinuclear complexes, CuEta, CuMep, and Cu(ℓ-Eph) have similar structures. Although these compounds and CuDiimH exhibit antiferromagnetic behavior, no simple correlation was found between the magnitude of antiferromagnetic coupling (2J) and the oxygen-oxygen distance of hydrogen bonds. It is also confirmed that there is no simple correlation between the 2J values and any single distance or angle. Several geometrical factors may, in combination, affect

the magnetic behavior, but it has not been possible to separate these in the compounds studied.

The oxygen-bridged tetramer, CoDeta, is the first 2,2′-dihydroxydiethylamine compound for which the structure has been solved. On the basis of M-O and M-N distances, interface cobalt atoms were assigned as divalent metal ions. The tetrameric units are connected into chains by hydrogen-bonding. This compound has weak antiferromagnetic coupling.

An oxygen-bridged dimer with a bent Cu_2O_2 ring, $CuPIPA \cdot 2H_2O$ shows weaker antiferromagnetic behavior than compounds with a planar Cu_2O_2 ring. The small Cu-O-Cu angles and the bent Cu_2O_2 ring support the molecular orbital explanation of weak antiferromagnetic coupling. One possible explanation for the discrepancy in the plot of magnetic susceptibilities versus temperature from theoretically predicted values of a copper dimer is additional coupling through the hydrogen-bonded water molecule network of this compound. An ESR spectroscopic study of the compound might be useful in further discussion of magnetic properties.

With this work, the study of widely varied hydrogen-bonded polynuclear units, hydrogen-bonded chains, or hydrogen-bonded networks in aminoalcohol and iminoalcohol transition metal complexes has just begun, but these studies indicate the importance of such interactions to an understanding of properties of the compounds. Hydrogen-bonded interactions in transition metal complexes may be very important in biological systems as well as in other systems. Further studies should be made on similar complexes to achieve a better understanding of the relationship between structures and magnetic properties of such complexes.

APPENDIX

Table A-1. Observed (FO) and Calculated (FC) Structure Factors for $Ni_2(Eta)_2(EtaH)_4(ClO_4)_2$

H	K	FO	FC
	L=	0	
4	0	74	74
8	0	22	23
10	0	27	28
16	0	24	26
4	1	117	120
6	1	14	12
10	1	15	11
12	1	19	17
4	2	59	56
6	2	20	18
8	2	26	25
10	2	11	11
14	2	13	10
4	3	35	36
8	3	70	68
12	3	19	18
14	3	25	24
2	4	30	30
4	4	65	64
6	4	58	56
10	4	25	24
12	4	32	30
14	4	17	17
2	5	14	13
4	5	22	23
6	5	37	35
8	5	18	15
10	5	16	17
12	5	12	9
4	6	53	53
6	6	50	47
10	6	37	38
2	7	77	76
4	7	28	27
6	7	11	8
8	7	35	34
12	7	14	14
14	7	12	13
2	8	20	19
4	8	15	13
2	9	36	35
4	9	25	25
6	9	23	23
8	9	20	22
12	9	17	17
2	10	13	10
4	10	26	26
6	10	33	34
10	10	24	24
12	10	12	12
4	11	21	20
6	11	12	12
10	11	13	11
2	12	16	12
4	12	23	24
6	12	12	10
10	12	15	16
4	13	10	7
8	13	25	26
2	14	13	10
4	14	15	16
6	14	12	6
4	15	13	12
6	15	11	9
	L=	1	
4	1	14	16
5	1	53	53
6	1	30	28
7	1	14	8
8	1	32	31
9	1	29	30
11	1	15	15
14	1	11	7
15	1	14	14
3	2	49	54
4	2	52	52
6	2	32	33
7	2	47	45
9	2	33	31
10	2	16	16
12	2	12	10
13	2	18	19
15	2	12	7
2	3	23	24
3	3	30	31
5	3	9	10
6	3	24	24
7	3	14	14
8	3	15	18
10	3	10	8
11	3	13	11
2	4	27	26
3	4	43	44
5	4	13	14
6	4	39	40
7	4	34	33
8	4	10	9
9	4	25	25
10	4	16	15
13	4	14	14
2	5	43	43
3	5	17	17
4	5	47	47
5	5	54	53
6	5	31	30
7	5	41	40
9	5	22	22
10	5	20	20
11	5	22	22
12	5	22	22
15	5	14	14
2	6	12	15
3	6	42	42
4	6	13	14
5	6	24	25
6	6	26	27
7	6	13	10
10	6	20	20
13	6	14	11
2	7	28	29
5	7	34	33
6	7	22	20
8	7	35	35
10	7	23	21
11	7	16	19
2	8	22	19
3	8	48	46
4	8	40	40
6	8	13	9
7	8	32	32
9	8	16	19
12	8	18	19
13	8	14	12
2	9	13	12
5	9	21	21
6	9	17	18
8	9	35	35
9	9	12	7
11	9	16	13
3	10	16	16
10	10	15	13
3	11	24	12
4	11	20	19
5	11	26	27
6	11	23	22
7	11	16	14
9	11	13	11
10	11	12	12
11	11	14	14
12	11	11	11
3	12	22	23
6	12	13	12
7	12	12	12
9	12	13	12
14	12	12	12
3	14	17	18
4	14	11	9
6	14	11	8
2	15	14	11
4	15	11	6
5	15	12	12
	L=	2	
3	2	31	33
5	2	22	21
6	2	26	27
7	2	39	40
9	2	26	25
10	2	15	13
11	2	12	11
14	2	13	9
16	2	11	9
3	3	29	29
4	3	56	55
5	3	66	67
6	3	30	30
7	3	22	21
8	3	10	10
9	3	29	30
10	3	19	20
12	3	20	21
15	3	14	15
3	4	18	19
4	4	13	13
5	4	31	32
6	4	16	18
7	4	48	48
9	4	27	28
10	4	17	16
11	4	12	10
13	4	17	16
3	5	21	22
5	5	22	20
7	5	10	10
8	5	11	9
3	6	88	87
4	6	12	14
6	6	13	13
7	6	26	26
9	6	18	19
10	6	12	7
12	6	14	8
13	6	19	18
5	7	48	50
7	7	23	23
8	7	18	19
9	7	18	17
11	7	19	20
3	8	12	12
8	8	11	8
3	9	13	12
5	9	30	29
7	9	12	10
8	9	12	11
9	9	17	17
11	9	15	15
3	10	42	42
4	10	20	20
6	10	10	11
7	10	17	17
9	10	19	20
13	10	13	14
6	11	13	8
7	11	13	10
3	12	14	15
7	12	13	12
4	13	13	12
5	13	23	25
6	13	14	16
9	13	12	5
3	14	15	16
	L=	3	
4	3	15	11
5	3	46	45
6	3	17	17
8	3	10	9
9	3	11	10
10	3	12	11
4	4	38	40
6	4	17	18
7	4	34	34
10	4	24	26
12	4	17	18
13	4	11	6
14	4	13	14
4	5	32	32
7	5	13	16
8	5	70	73
9	5	19	19
12	5	14	12
14	5	15	16
4	6	50	51
5	6	10	9
6	6	10	9
10	6	9	4
12	6	16	16
4	7	28	30
5	7	19	18
6	7	32	33
10	7	17	17
12	7	15	14
4	8	39	39
5	8	28	29
6	8	42	43
10	8	27	27
4	9	34	36
5	9	17	18
6	9	24	24
9	9	13	13
10	9	14	11
12	9	13	10
4	10	21	19
4	11	18	19
8	11	22	24
9	11	10	9
4	12	18	19
6	12	13	14
7	12	10	7
10	12	13	9
5	13	11	6
4	14	11	13
6	14	15	11
4	15	13	11
	L=	4	
4	4	51	50
5	4	24	23
6	4	21	20
7	4	34	36
9	4	17	17
10	4	21	23
13	4	17	19
5	5	11	8
6	5	22	21
7	5	12	8
8	5	23	22
9	5	13	16
11	5	12	7
5	6	19	17
6	6	44	41
7	6	27	28
9	6	18	18
10	6	15	17
11	6	13	11
12	6	11	9
13	6	12	8
5	7	29	29
7	7	11	9
8	7	15	15
9	7	15	15
11	7	12	10
12	7	13	10
14	7	12	6
7	8	10	6
5	9	22	24
8	9	10	15
11	9	12	9
12	9	11	8
5	10	13	10
6	10	18	19
7	10	16	17
10	10	12	12
5	11	12	10
8	11	12	10
10	11	12	9
5	12	10	9
5	13	11	9
6	13	14	10
7	13	11	6
9	13	14	14
5	15	14	7
	L=	5	
5	5	68	66
9	5	12	14
11	5	31	34
6	6	15	15
7	6	23	20
9	6	14	15
11	6	11	6
7	7	24	28
9	7	20	20
7	8	24	23
9	8	16	16
13	8	20	19
7	9	23	24
8	9	15	17
9	9	16	15
9	11	12	9
10	11	11	3
11	11	16	17
7	12	15	14
9	12	13	12
	L=	6	
6	6	27	25
7	6	16	15
8	6	11	8
9	6	14	16
10	6	15	19
8	7	27	27
10	7	13	9
11	7	13	11
12	7	14	13
7	8	11	8
8	9	17	17
12	9	12	10
7	10	13	13
10	10	17	16
8	13	14	15
	L=	7	
7	7	18	17
8	7	18	18
11	7	13	11
9	8	12	11
10	8	16	16
12	8	14	11
8	9	13	12
11	9	12	9
8	11	14	17
9	11	12	8
	L=	8	
9	9	12	13
9	10	13	14

Table A-2. Observed (FO) and Calculated (FC) Structure Factors for $[Cu(Eta)(EtaH)]_2(NO_3)_2$

K	L	FO	FC
	H= -11		
2	1	19	19
2	2	8	7
2	3	17	17
3	0	5	4
3	1	18	19
3	2	8	8
3	3	9	10
4	0	11	10
4	1	21	21
4	2	9	9
4	3	8	9
5	0	15	14
5	1	16	15
5	2	5	5
5	3	10	11
6	0	13	13
6	1	15	15
6	2	5	4
6	3	10	10
7	0	11	11
7	1	21	21
7	2	9	8
7	3	14	15
8	0	14	14
8	1	20	20
8	2	13	13
8	3	14	18
9	0	8	7
9	1	19	19
9	2	12	11
10	0	6	4
	H= -10		
0	1	4	5
0	3	19	19
0	4	7	6
0	5	22	21
1	3	16	16
1	4	7	6
1	5	23	22
2	0	5	5
2	1	10	10
2	3	21	22
2	4	11	10
2	5	23	23
2	6	11	10
3	0	8	8
3	3	21	22
3	4	9	4
3	5	21	19
3	6	13	12
4	2	6	6
4	3	7	9

K	L	FO	FC
	H= -11		
4	5	18	18
4	6	11	10
5	1	8	6
5	2	8	7
5	3	5	7
5	4	5	5
5	5	20	20
5	6	8	7
6	0	4	4
6	3	22	23
6	4	6	5
6	5	23	22
7	3	19	19
7	4	6	6
7	5	23	23
8	0	3	4
8	1	11	11
8	2	5	3
8	3	10	10
8	4	7	7
9	1	13	12
9	3	16	16
10	1	5	4
11	0	5	5
	H= -9		
-2	1	12	13
-2	2	6	7
-2	3	9	9
-2	5	4	3
-1	0	13	13
-1	1	24	24
-1	2	13	12
-1	3	12	10
-1	6	12	12
0	0	12	12
0	1	28	28
0	2	21	21
0	3	15	14
0	4	4	6
0	5	8	10
0	6	16	16
0	7	7	8
1	1	25	24
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8	2	19	19
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9	3	18	16
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-1	6	17	17
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0	3	6	5
0	4	20	20
0	6	23	22
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0	8	6	5
1	0	19	20
1	1	10	9
1	2	8	7
1	3	12	12
1	4	33	34
1	5	5	6
1	6	24	23
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2	0	25	26
2	1	4	5
2	2	15	15
2	3	18	17
2	4	38	40
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2	6	23	23
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3	3	4	4
3	4	33	35
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3	6	25	24
3	8	7	8
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4	2	5	4
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4	4	33	34
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4	8	6	6
5	0	11	12

K	L	FO	FC
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5	3	16	14
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5	6	20	21
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6	3	9	7
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6	7	7	7
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7	2	12	14
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7	5	6	6
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8	3	8	6
8	4	30	30
8	5	8	8
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9	2	8	8
9	3	6	5
9	4	16	18
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12	0	12	11
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0	8	15	14
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1	2	47	45
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2	1	3	6
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2	5	10	11
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3	2	55	57
3	4	38	38
3	6	12	12
3	7	14	14
3	8	23	22
3	9	13	13
4	0	18	18
4	1	8	5

K	L	FC	FC
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4	6	5	6
4	7	13	13
4	8	24	24
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5	2	54	53
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5	7	10	11
5	8	18	18
6	0	31	31
6	1	8	9
6	2	32	32
6	3	12	11
6	4	20	20
6	5	4	4
6	7	8	8
7	0	19	19
7	1	12	12
7	2	23	23
7	3	3	3
7	4	21	22
7	6	4	4
7	7	6	5
8	0	23	23
8	1	7	7
8	2	45	45
8	3	8	7
8	4	29	29
8	6	5	5
9	0	21	20
9	2	36	37
9	4	24	24
9	5	4	3
10	0	15	15
10	1	3	2
10	2	24	24
10	4	14	14
11	0	8	8
12	0	8	9
12	1	8	7
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-6	3	10	11
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-6	5	18	18
-6	6	10	10
-6	7	8	7
-5	0	20	19

K	L	FO	FC
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-1	4	9	9
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-1	8	10	10
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0	2	9	7
0	3	11	12
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0	6	36	35
0	7	13	14
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0	9	6	7
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Table A-2. (Continued)

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2	7	21	20
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3	2	12	12
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3	5	25	24
3	6	36	35
3	7	20	22
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4	2	12	14
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9	0	32	30
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1	10	6	5
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2	3	11	10
2	4	18	20
2	5	56	61
2	6	11	11
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2	8	19	18
2	9	4	4
2	10	8	7
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Table A-2. (Continued)

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-3	10	27	28
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-2	3	73	71
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-2	5	45	47
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0	1	45	42
0	2	24	27
0	3	74	75
0	4	52	53
0	5	3	1
0	6	3	3
0	8	30	29
0	9	19	15
0	10	15	14
0	11	7	7
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1	3	68	93
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1	5	40	41
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1	9	8	8
1	10	11	11
2	0	15	16
2	1	77	74
2	2	10	11
2	3	94	98
2	4	5	4
2	5	37	40
2	6	15	17
2	7	26	27
2	9	17	16
2	9	10	10
2	10	15	14
3	0	23	23
3	1	30	29
3	2	40	42
3	3	82	83
3	4	24	26
3	5	15	10
3	6	24	23
3	7	16	16
3	8	18	17
3	9	13	12
4	0	22	19
4	1	60	61
4	2	42	43
4	3	71	72
4	4	15	15
4	5	30	31
4	6	3	3
4	8	21	20
4	9	15	14
5	0	43	41
5	1	54	51
5	2	32	33
5	3	61	64
5	5	35	36
5	6	17	17
5	8	17	17
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7	3	39	40
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7	5	15	15
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8	1	29	26
8	3	28	29
8	4	8	8
8	5	23	24

K	L	FO	FC
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10	2	12	12
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11	1	13	12
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0	5	13	13
0	6	48	50
0	7	25	24

K	L	FO	FC
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1	4	35	36
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2	6	57	58
2	7	15	15
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3	3	15	15
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3	5	35	34
3	6	41	43
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3	8	27	28
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4	4	17	17
4	5	10	10
4	6	24	25
4	7	14	14
4	8	22	22
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5	2	16	17
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5	4	7	7
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6	3	34	35
6	4	14	14
6	5	6	7
6	6	14	15
6	7	10	10
7	0	25	26
7	1	46	50
7	2	32	33

K	L	FO	FC
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7	4	8	6
7	5	5	6
7	6	21	21
8	0	25	25
8	1	35	37
8	2	14	14
8	3	10	10
8	4	9	10
8	5	7	7
9	0	7	7
9	1	18	18
9	3	11	11
9	4	5	5
9	6	9	9
10	0	8	9
10	1	22	23
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10	3	6	5
11	0	14	14
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-8	8	21	20
-8	9	14	14
-7	0	11	13
-7	1	16	16
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-6	3	22	21
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-5	4	83	85
-5	5	24	24
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-4	5	11	11
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-2	5	16	15
-2	6	4	4
-2	7	10	12
-2	8	22	21
-2	9	16	17
-2	10	29	30
-2	11	10	10

K	L	FO	FC
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-1	3	30	28
-1	4	26	25
-1	5	12	10
-1	6	14	12
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-1	8	19	18
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-1	11	6	7
0	1	4	7
0	2	161	164
0	3	16	15
0	4	46	48
0	5	7	9
0	6	32	33
0	7	18	14
0	8	22	20
0	10	14	15
1	11	5	5
1	0	2	2
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1	3	29	28
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1	6	18	17
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1	10	19	19
1	8	15	15
1	9	7	8
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2	1	34	32
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2	6	12	11
2	7	9	8
2	8	17	14
2	9	9	9
2	11	22	23
3	0	27	27
3	1	41	39
3	2	87	87
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3	8	13	14
3	9	4	5

Table A-2 (Continued)

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5	1	7	8
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5	3	12	13
5	4	25	25
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8	2	16	16
8	3	8	8
8	4	34	35
9	1	4	4
9	2	15	14
9	3	10	9
9	4	27	27
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10	2	13	13
11	0	5	5

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-11	7	17	17
-11	8	11	10
-10	0	24	24
-10	1	5	4
-10	2	7	6
-10	4	12	13
-10	5	15	14
-10	6	24	24

K	L	FO	FC
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-9	0	10	10
-9	4	17	17
-9	5	8	8
-9	6	19	19
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-8	2	13	14
-8	3	11	12
-8	4	17	18
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-7	3	10	11
-7	5	21	21
-7	6	38	38
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-7	10	7	6
-7	11	8	7
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-6	7	22	22
-6	8	22	21
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-5	7	41	42
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-5	9	9	8
-5	11	12	10
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-4	6	57	56
-4	7	37	39
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K	L	FC	FC
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-2	7	30	31
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0	5	35	39
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0	8	25	27
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1	3	15	14
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1	5	19	17
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1	8	24	25
1	9	9	8
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2	1	24	21
2	2	28	26
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2	4	20	22

K	L	FO	FC
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3	8	15	16
3	9	11	11
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6	6	22	21
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7	5	6	5
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9	2	24	25
9	3	7	6
10	0	24	24

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-11	1	6	7
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-11	3	21	21

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-11	8	10	10
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-10	2	14	15
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-6	11	20	20
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-5	3	81	81

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-3	11	22	22
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-2	1	33	30
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0	2	65	60
0	3	46	48
0	4	60	62
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K	L	FC	FC
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0	9	20	19
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1	1	47	45
1	2	46	45
1	3	60	61
1	4	54	53
1	5	50	50
1	6	16	16
1	9	23	24
2	0	29	26
2	1	57	54
2	2	73	71
2	3	51	52
2	4	47	47
2	5	35	34
2	6	9	9
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2	9	9	10
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3	1	16	16
3	2	38	39
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3	8	13	14
4	0	7	7
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4	2	17	17
4	3	37	37
4	4	28	26
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4	6	7	7
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5	1	13	13
5	2	28	28
5	3	36	36
5	4	28	27
5	5	13	13
5	6	11	11
6	0	33	34
6	1	12	13
6	2	21	20
6	3	18	18
6	4	23	24
6	5	20	20
6	7	30	32
6	8	6	9
7	0	12	13
7	1	4	3
7	2	13	14
7	3	10	10

K	L	FO	FC
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7	5	16	16
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8	2	15	15
8	3	12	12
9	0	9	10
9	1	5	5
9	2	8	8
10	0	9	9

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K	L	FO	FC
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-11	1	19	18
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-11	5	22	22
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-9	4	24	22
-9	5	34	33
-9	6	5	6
-9	7	43	44
-9	8	12	10
-9	9	20	20
-9	10	4	3
-9	11	9	9
-8	0	26	25
-8	1	61	53
-8	2	23	30
-8	4	12	11
-8	5	37	35
-8	6	6	8
-8	7	30	32
-8	8	6	9
-8	9	22	21
-8	11	10	8
-7	0	24	26
-7	1	45	46

Table A-2. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
-7	2	23	24	-2	6	3	1	5	1	59	58	-9	4	8	8	-4	6	11	8	2	0	23	20	-10	2	15	14	-5	8	35	35
-7	3	9	8	-2	7	53	56	5	2	28	29	-9	5	35	36	-4	7	3	1	2	1	3	3	-10	3	22	22	-5	9	4	5
-7	4	15	17	-2	9	24	23	5	3	16	18	-9	6	14	14	-4	8	11	9	2	2	14	15	-10	4	6	5	-5	10	9	8
-7	5	34	31	-1	0	49	48	5	5	7	7	-9	8	14	12	-4	9	16	17	2	3	48	44	-10	5	14	14	-4	0	16	18
-7	6	3	5	-1	1	143	144	6	0	26	27	-9	9	16	15	-4	10	21	21	2	4	8	8	-10	6	35	35	-4	1	58	58
-7	7	30	31	-1	2	60	63	6	1	38	37	-9	10	15	15	-4	11	13	14	2	5	47	49	-10	7	14	13	-4	2	22	20
-7	8	8	10	-1	3	26	21	6	2	13	13	-9	11	16	18	-3	0	24	23	2	6	14	13	-10	8	28	30	-4	3	40	41
-7	9	25	24	-1	4	22	27	6	3	17	16	-8	0	12	13	-3	1	17	18	2	7	9	8	-10	10	6	6	-4	5	3	3
-7	11	7	7	-1	5	26	22	6	4	7	8	-8	1	19	19	-3	2	72	66	3	1	12	13	-9	0	18	20	-4	6	43	42
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-3	6	14	14	3	6	11	11	-10	3	33	32	-5	5	52	57	0	7	8	7	-12	9	5	4	-6	7	34	30	0	1	107	105
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-3	9	28	27	4	1	48	49	-10	6	10	9	-5	10	6	8	1	1	20	21	-11	2	19	18	-5	0	44	46	0	4	5	2
-3	11	5	5	4	2	38	39	-10	7	6	8	-5	11	8	8	1	2	14	13	-11	3	9	9	-5	1	93	90	0	5	8	11
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-2	3	15	11	4	6	5	5	-9	1	15	15	-4	3	86	82	1	6	19	19	-11	8	31	32	-5	5	13	15	0	9	6	6
-2	4	46	38	4	7	23	23	-9	2	28	28	-4	4	15	20	1	7	5	4	-10	0	12	12	-5	6	43	40	1	0	36	36
-2	5	43	39	5	0	34	34	-9	3	41	40	-4	5	74	79	1	9	10	9	-10	1	22	22	-5	7	30	29	1	1	96	96

Table A-2. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
1	2	34	34	-10	3	10	8	-4	7	6	6	6	1	6	5	-7	8	22	23	-1	7	6	5	-10	4	25	26	-3	0	29	29
1	3	15	15	-10	4	40	41	-4	9	7	6		H=	6		-7	9	4	4	-1	8	17	16	-10	5	23	22	-3	1	11	11
1	4	11	9	-10	6	22	22	-4	10	21	21					-7	10	13	13	0	0	60	58	-10	6	23	23	-3	2	23	24
1	5	20	18	-10	10	22	22	-3	0	9	7					-6	0	74	71	0	1	3	3	-10	7	14	15	-3	3	12	12
1	6	20	19	-9	0	3	2	-3	1	21	19	-13	2	22	22	-6	1	14	14	0	2	52	54	-10	8	8	8	-3	4	26	26
1	7	23	22	-9	2	12	11	-3	2	15	14	-13	6	14	14	-6	2	60	59	0	4	11	10	-10	9	9	8	-3	5	16	16
1	8	14	14	-9	3	30	30	-3	3	29	30	-13	7	14	14	-6	3	11	11	0	5	12	12	-9	0	20	20	-3	6	23	22
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2	6	16	14	-9	9	6	7	-2	2	12	9	-12	8	16	16	-6	9	7	7	1	3	4	5	-9	6	19	19	-2	3	31	32
2	7	16	15	-9	10	21	22	-2	3	35	37	-11	0	30	30	-6	10	11	10	1	4	16	17	-9	7	14	14	-2	4	10	12
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4	2	14	14	-8	10	19	20	-1	3	6	9	-10	2	15	16	-5	8	23	24	3	1	3	2	-8	6	20	19	-1	4	27	27
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	H=	5		-6	5	14	13	1	4	38	39	-9	9	15	15	-3	4	11	11	-13	6	7	7	-6	2	26	26	2	0	19	19
				-6	6	40	41	1	5	12	12	-9	10	7	7	-3	5	5	4	-12	0	9	9	-6	4	32	31	2	4	16	16
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-10	1	7	5	-4	5	15	13	5	3	11	11	-7	6	33	33	-1	4	12	13	-10	2	20	20	-4	7	19	19	-12	7	15	16
-10	2	6	6	-4	6	36	37	6	0	16	16	-7	7	20	20	-1	6	24	23	-10	3	16	16	-4	8	7	7	-11	8	7	8

Table A-2. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC	K	L	FJ	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
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-11	2	19	18	-3	1	22	22	-8	6	7	6	-10	4	4	4	-6	3	5	5												
-11	3	20	19	-3	2	27	28	-8	7	7	7	-10	6	4	4	-6	4	10	10												
-11	4	7	8	-3	3	22	21	-7	0	5	5	-9	1	15	16	-5	0	15	14												
-11	5	7	6	-3	4	19	19	-7	1	18	17	-9	2	6	6	-5	1	9	10												
-11	6	4	3	-3	6	4	3	-7	3	23	21	-9	3	13	14	-5	2	4	6												
-11	7	22	23	-3	7	15	15	-7	5	29	29	-9	4	5	4	-5	3	5	7												
-10	0	11	11	-2	0	25	26	-7	6	6	6	-8	1	22	23	-4	0	10	10												
-10	1	27	26	-2	1	26	27	-7	7	8	9	-8	2	7	9	-4	1	8	9												
-10	2	20	20	-2	2	16	17	-6	0	13	13	-8	3	19	20	-3	0	6	4												
-10	3	25	24	-2	3	22	21	-6	1	12	12	-8	4	12	9	-3	1	7	6												
-10	4	15	13	-2	4	14	13	-6	3	20	18	-7	1	33	34																
-10	7	27	27	-2	6	6	6	-6	4	7	6	-7	2	13	14																
-9	0	19	19	-1	0	18	20	-6	5	25	26	-7	3	30	30																
-9	1	22	24	-1	1	20	21	-6	7	12	11	-7	4	12	12																
-9	2	10	12	-1	2	17	17	-5	0	21	20	-6	0	4	4																
-9	3	21	21	-1	3	24	23	-5	1	8	7	-6	1	31	31																
-9	4	16	16	-1	5	6	5	-5	3	23	21	-6	2	14	16																
-9	7	18	19	0	0	19	20	-5	4	8	8	-6	3	25	26																
-8	0	23	24	0	1	16	16	-5	5	27	29	-6	4	9	8																
-8	1	26	26	0	2	25	25	-5	6	4	5	-5	1	30	31																
-8	2	24	24	0	3	24	22	-5	7	17	17	-5	2	6	7																
-8	3	21	20	1	0	7	8	-4	0	13	13	-5	3	17	18																
-8	4	7	4	1	1	15	15	-4	1	20	20	-5	4	4	4																
-8	5	10	9	1	2	18	17	-4	3	10	9	-4	1	22	22																
-8	6	8	8	1	3	21	20	-4	5	27	28	-4	2	4	4																
-8	7	13	15	2	0	5	5	-4	6	9	9	-4	3	14	15																
-7	0	23	24	2	1	10	11	-3	0	5	4	-4	4	10	9																
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-7	2	30	32	3	0	9	9	-3	3	4	2	-3	1	12	13																
-7	3	37	36					-3	5	22	23	-3	3	10	11																
-7	5	4	4		H=	9		-2	1	4	5	-3	4	7	8																
-7	6	5	4					-2	2	5	3	-2	0	4	5																
-7	7	12	13	-12	0	8	8	-2	3	9	8	-2	1	17	17																
-6	0	29	28	-12	3	19	18	-2	4	5	5	-2	3	16	17																
-6	1	24	26	-12	5	21	22	-2	5	18	19	-1	1	19	19																
-6	2	27	28	-11	0	11	10	-1	1	15	16	-1	2	7	7																
-6	3	35	33	-11	1	6	5	-1	3	8	8																				
-6	4	11	13	-11	3	17	16	-1	4	6	6		H=	11																	
-6	5	4	6	-11	5	23	24	0	0	12	12																				
-6	6	9	9	-11	6	11	10	0	1	16	15	-10	0	6	4																
-6	7	12	14	-11	7	14	14	0	3	8	7	-10	3	6	7																
-5	0	11	12	-10	0	6	7	1	0	13	13	-9	0	8	7																
-5	1	31	30	-10	1	4	5	1	1	10	10	-9	1	9	8																
-5	2	23	30	-10	3	13	10					-9	4	16	15																
-5	3	35	32	-10	5	29	31		H=	10		-8	0	14	14																
-5	5	4	3	-10	6	6	6					-8	1	10	10																
-5	6	4	5	-10	7	11	11	-12	2	12	12	-8	3	4	7																
-5	7	20	21	-9	0	4	3	-12	3	15	15	-8	4	14	15																
-5	8	5	5	-9	2	3	3	-11	0	4	5	-7	0	11	11																
-4	0	4	5	-9	3	6	6	-11	1	22	22	-7	1	12	12																
-4	1	28	29	-9	5	25	27	-11	2	10	10	-7	2	4	5																
-4	2	29	30	-9	6	5	4	-11	3	11	11	-7	3	8	9																
-4	3	33	33	-9	7	9	8	-11	4	9	8	-7	4	14	14																
-4	4	10	10	-8	3	20	18	-10	1	19	20	-6	0	13	13																
-4	7	20	20	-8	4	8	7	-10	2	4	3	-6	1	12	12																

Table A-3. Observed (FO) and Calculated (FC) Structure Factors for $[Cu(Mep)(MepH)(H_2O)]_2(NO_3)_2$

K	L	FO	FC
	H= -8		
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0	6	11	9
0	10	13	10
1	8	13	11
1	11	12	9
2	1	14	12
2	3	10	5
2	7	13	12
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4	12	12	10
4	14	11	8
5	5	11	11
5	7	12	8
6	6	12	9
7	9	13	11
	H= -7		
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0	6	20	16
0	9	12	11
0	12	12	11
0	14	13	10
1	4	17	17
1	7	12	12
1	12	10	8
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6	11	12	12
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8	9	12	8
8	14	11	11
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9	5	12	12
9	13	12	9
9	14	11	3
10	7	11	3
11	4	11	10
11	6	12	8
	H= -6		
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0	2	26	25
0	4	34	33
0	6	24	25
0	8	29	27
0	10	21	20
0	12	21	22
0	16	14	13
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12	1	11	8
12	7	17	15
12	8	11	7
13	3	12	10
13	5	13	11
13	9	13	11
	H= -5		
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0	2	8	8
0	4	36	35
0	6	35	35
0	8	29	30
0	10	14	16
0	12	15	16
0	14	25	26
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0	20	16	16
1	0	9	9
1	1	24	24
1	2	46	45
1	4	19	21
1	5	37	38
1	7	27	27
1	8	18	19
1	10	34	34
1	11	19	17
1	12	16	15
1	13	24	21
1	16	22	21
1	18	17	16
1	19	13	11
2	1	25	25
2	3	41	41
2	4	9	4
2	5	13	14
2	6	23	23
2	7	25	25
2	9	37	37
2	10	11	9
2	11	35	34
2	15	25	24
2	17	22	20
2	19	11	11
3	0	13	13
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4	2	23	25
4	3	13	13
4	4	13	10
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4	8	15	15
4	10	11	12
4	12	23	23
4	14	13	10
4	20	16	16
5	0	8	7
5	1	17	17
5	2	9	8
5	4	10	9
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5	6	15	16
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5	19	14	13
5	21	15	11
6	0	13	14
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6	12	14	13
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7	1	13	13
7	2	32	32
7	3	18	17
7	4	23	26
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7	8	25	28
7	10	34	33
7	12	13	13
7	16	19	18
7	18	14	16
8	0	33	32
8	1	12	11
8	2	16	15
8	3	15	16
8	4	17	16
8	6	24	24
8	7	24	24
8	8	22	23
8	9	17	17
8	11	17	14
8	12	11	10
8	14	14	14
8	15	12	11
9	1	22	21
9	5	27	26
9	7	21	19
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14	2	13	10
14	6	20	19
14	12	13	11
15	5	14	8
15	10	17	13
16	3	15	11
	H= -4		
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0	2	67	68
0	4	31	33
0	6	18	20
0	8	52	53
0	10	17	18
0	14	39	39
0	16	29	29
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1	4	33	34
1	5	18	18
1	6	49	49
1	7	26	26
1	8	18	18
1	9	38	38
1	12	27	27
1	14	15	15
1	15	28	28
1	17	14	13
1	20	11	11
1	21	13	14
2	1	34	34
2	3	7	7
2	4	22	22
2	5	36	37
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2	7	34	34
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2	9	12	13
2	11	24	24
2	12	12	10
2	13	30	30
2	16	10	10
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2	21	12	10
3	0	26	27
3	1	12	13
3	4	23	24
3	5	10	11
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3	7	27	27
3	8	27	28
3	9	9	12
3	11	28	29
3	12	19	21
3	13	12	13
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3	15	12	12
3	17	17	16
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5	15	17	17
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5	18	15	13
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6	11	29	31
6	12	17	11
6	13	31	32
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7	7	9	10
7	9	15	16
7	12	33	33
7	14	15	12
7	20	14	14
8	2	29	30
8	3	9	7
8	4	16	15
8	5	19	18

Table A-3 (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC
8	9	30	32	14	10	20	18	2	23	13	13	6	12	21	21	11	2	31	32	0	22	19	20	4	3	9	8	7	13	10	10
9	13	25	27	14	14	15	11	3	0	20	20	6	13	20	22	11	4	16	14	1	0	38	39	4	4	9	9	7	14	14	15
9	17	12	10	15	0	19	18	3	1	14	14	6	14	21	22	11	6	12	9	1	1	97	95	4	5	22	22	7	19	39	28
8	14	22	22	15	1	14	9	3	2	61	64	6	15	23	24	11	7	10	9	1	2	77	77	4	8	51	54	7	20	12	12
8	16	15	17	15	4	16	16	3	3	7	5	6	17	20	19	11	8	12	10	1	3	27	27	4	10	22	23	7	21	9	9
9	0	11	10	15	6	23	23	3	4	39	40	6	18	12	11	11	10	14	15	1	4	136	140	4	11	25	24	8	0	46	47
9	1	33	33	15	12	22	18	3	5	49	50	6	21	14	14	11	14	21	20	1	5	51	51	4	12	10	12	8	1	13	14
9	5	22	21	16	5	19	17	3	6	26	26	7	0	36	36	11	16	13	15	1	6	68	68	4	14	38	37	8	2	64	65
9	6	16	15	16	11	13	13	3	7	20	20	7	1	15	14	12	1	27	26	1	7	66	69	4	16	32	32	8	3	53	53
9	7	20	21					3	8	45	45	7	2	65	63	12	3	30	29	1	9	49	50	4	20	15	15	8	4	15	15
9	8	12	12			H= -3		3	9	15	16	7	3	29	30	12	4	27	26	1	10	54	55	4	22	15	16	8	5	27	27
9	9	38	37					3	10	39	40	7	4	26	25	12	6	19	19	1	12	61	64	5	0	13	12	8	6	18	18
9	11	16	16	0	0	46	45	3	11	18	17	7	6	20	20	12	9	24	24	1	13	31	31	5	1	83	80	8	7	9	10
9	13	10	13	0	2	8	5	3	13	19	20	7	7	14	14	12	11	11	10	1	14	17	17	5	2	30	28	8	8	42	42
9	15	25	24	0	4	163	165	3	14	32	33	7	8	41	42	12	12	19	19	1	15	38	40	5	3	60	58	8	9	28	28
9	17	16	15	0	6	70	74	3	16	14	13	7	9	13	13	12	15	13	13	1	16	13	14	5	4	24	23	8	10	26	25
10	1	24	24	0	8	72	73	3	18	20	21	7	10	33	34	12	17	13	10	1	18	18	20	5	5	50	50	8	11	35	35
10	2	21	21	0	10	47	48	3	19	14	16	7	11	20	20	13	2	19	20	1	19	13	14	5	6	9	11	8	12	27	22
10	5	11	14	0	12	52	54	4	0	55	55	7	14	25	25	13	3	22	20	1	20	16	15	5	7	30	32	8	13	14	13
10	7	25	24	0	14	54	56	4	1	22	23	7	16	31	32	13	5	31	30	1	21	19	17	5	8	51	52	8	14	19	20
10	9	10	11	0	18	19	20	4	2	19	18	8	0	21	21	13	7	13	14	2	1	28	29	5	10	17	16	9	15	11	10
10	10	13	12	0	20	17	15	4	3	29	28	8	1	36	36	13	8	11	10	2	2	28	27	5	12	13	12	9	16	19	18
10	13	14	12	1	0	12	12	4	4	44	47	8	2	16	17	13	10	12	14	2	3	91	91	5	13	38	37	9	17	25	24
10	14	12	12	1	1	53	52	4	5	22	23	9	3	37	36	13	11	25	24	2	4	41	41	5	14	9	8	8	19	19	17
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11	0	21	19	1	4	20	20	4	8	9	9	8	6	39	39	14	0	16	17	2	7	39	41	5	17	23	23	9	0	17	17
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11	4	27	26	1	7	44	45	4	12	46	48	8	9	23	24	14	10	11	9	2	11	70	74	5	23	15	14	9	6	11	10
11	6	25	25	1	8	9	10	4	13	17	17	8	10	26	27	14	12	16	17	2	13	36	37	6	0	31	30	9	7	45	45
11	7	10	13	1	9	11	10	4	20	14	13	8	11	18	18	15	0	19	19	2	14	17	18	6	1	17	17	9	8	15	16
11	9	17	18	1	10	28	30	5	0	9	9	8	12	24	25	15	2	21	19	2	16	12	13	6	2	41	42	9	9	44	44
11	12	10	14	1	11	35	37	5	1	24	24	8	13	17	18	15	6	12	11	2	17	29	29	6	3	87	88	9	13	17	18
11	14	18	17	1	12	12	12	5	2	19	18	8	14	20	19	15	8	21	22	2	19	31	31	6	5	71	69	9	15	25	24
11	17	11	8	1	13	29	30	5	3	27	27	8	21	13	10	15	10	16	16	2	21	12	8	6	6	26	24	9	17	9	11
12	1	21	20	1	14	14	15	5	4	7	8	9	0	10	10	15	14	15	14	3	0	47	44	6	8	19	19	9	21	14	15
12	2	13	14	1	15	12	10	5	5	67	66	9	1	24	24	16	1	17	18	3	1	31	32	6	9	23	22	10	0	24	24
12	3	9	7	1	16	29	31	5	6	39	37	9	3	32	32	16	3	20	19	3	2	62	62	6	10	18	18	10	2	25	25
12	5	21	21	1	17	18	18	5	7	33	33	9	5	45	45	16	7	14	13	3	3	9	9	6	11	63	66	10	3	21	21
12	7	11	13	1	19	13	12	5	8	19	20	9	6	9	6	16	9	15	13	3	4	41	44	6	12	11	11	10	5	27	26
12	8	11	12	1	22	13	13	5	9	15	14	9	7	31	31	17	3	12	10	3	5	17	18	6	13	25	28	10	6	13	11
12	11	15	13	2	0	22	22	5	11	43	44	9	11	32	33	17	5	15	14	3	6	26	28	6	14	16	16	10	7	20	20
12	13	20	19	2	1	64	65	5	13	40	42	9	13	21	29	18	4	19	16	3	7	10	11	6	16	11	13	10	9	22	22
13	1	14	15	2	3	62	65	5	14	23	23	9	19	12	14					3	8	7	8	6	17	16	16	10	9	12	12
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Table A-3 (Continued)

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Table A-3. (Continued)

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8	17	25	25
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1	19	14	15
2	1	41	42
2	2	36	34
2	3	70	71
2	5	60	59
2	6	36	35
2	7	22	23
2	8	15	15
2	9	21	21
2	11	20	19
2	12	20	21
2	13	8	6
2	15	28	28
2	17	16	17
3	0	45	44
3	1	30	29
3	2	7	5
3	4	52	51
3	5	53	52
3	6	7	7
3	7	14	14
3	8	13	13
3	10	12	11
3	11	14	14
3	13	23	23
3	14	24	24
3	15	8	9
3	16	19	20
3	19	8	5
3	20	9	6
4	0	36	37
4	1	10	10
4	2	8	9
4	3	12	12
4	4	59	59
4	5	15	14
4	6	58	60
4	7	14	13
4	9	43	43
4	9	8	10
4	10	9	10
4	12	26	27
4	14	18	19
5	0	13	12
5	1	41	41
5	2	6	6
5	4	15	16
5	5	38	39
5	6	6	5
5	7	39	39
5	8	9	9
5	10	23	22
5	11	10	11
5	12	14	15
5	13	23	23
5	14	11	12
5	15	15	15
5	16	9	10
6	0	30	30
6	1	49	51
6	2	9	11
6	3	52	53
6	5	14	15
6	6	20	20
6	7	29	28
6	8	11	11
6	9	50	51
6	10	8	5

Table A-3 (Continued)

K	L	FO	FC
6	11	17	17
6	14	10	11
6	15	29	29
6	17	15	17
7	0	34	35
7	1	37	38
7	2	51	52
7	3	16	17
7	4	47	48
7	5	15	15
7	6	9	9
7	7	23	23
7	8	48	49
7	10	31	32
7	12	12	12
7	14	21	20
7	15	11	10
7	16	29	30
8	0	46	47
8	1	21	21
8	2	10	9
8	3	42	41
8	4	40	39
8	5	43	43
8	6	76	76
8	7	7	5
8	8	18	17
8	9	10	11
8	11	16	17
8	12	23	23
8	14	31	32
8	15	13	12
8	17	3	6
9	0	17	17
9	1	16	16
9	3	13	13
9	5	58	59
9	7	34	35
9	10	9	8
9	11	25	26
9	13	37	36
9	14	6	7
9	15	12	12
10	0	23	24
10	1	21	22
10	2	14	15
10	3	21	21
10	4	17	18
10	5	21	21
10	6	24	25
10	9	3	9
10	11	11	9
10	12	10	9
10	13	9	8
10	14	10	8
10	15	8	7

K	L	FO	FC
11	0	11	11
11	1	15	16
11	2	18	18
11	4	17	16
11	5	8	8
11	6	9	7
11	9	22	23
11	10	19	19
11	11	9	10
11	16	11	11
12	0	15	15
12	1	29	29
12	3	15	15
12	4	21	22
12	5	7	8
12	6	16	16
12	7	14	14
12	8	15	16
12	9	21	22
12	10	10	9
12	12	11	10
12	15	12	13
13	0	15	16
13	1	17	16
13	3	10	8
13	5	29	30
13	7	29	29
13	11	11	12
13	13	20	19
13	15	14	12
14	0	27	26
14	1	10	12
14	3	19	20
14	4	21	20
14	6	36	37
14	7	11	10
14	9	13	14
14	12	17	16
14	14	17	16
15	0	9	9
15	2	24	24
15	4	21	20
15	8	18	18
15	10	11	12
15	11	9	6
15	1	16	15
15	2	8	6
16	3	22	23
16	4	10	8
16	5	9	7
16	6	14	14
16	7	11	12
16	9	14	15
16	11	14	10
17	2	9	10
17	5	12	12

K	L	FO	FC
17	7	9	11
17	8	9	10
18	9	10	9
18	6	13	12
	M=	3	
0	0	44	45
0	2	110	114
0	4	82	83
0	6	24	24
0	8	60	60
0	10	64	66
0	14	22	23
0	16	24	24
0	18	16	16
1	0	12	12
1	1	63	62
1	2	13	12
1	3	65	64
1	4	67	68
1	5	30	29
1	6	31	31
1	7	31	32
1	8	18	18
1	9	41	42
1	10	24	24
1	11	16	17
1	12	22	23
1	14	10	9
1	15	19	19
1	17	14	13
1	1=	11	11
2	0	22	22
2	1	5	6
2	2	16	16
2	3	43	43
2	4	24	24
2	5	72	71
2	6	6	4
2	7	28	28
2	8	7	7
2	9	14	14
2	11	29	29
2	13	40	40
2	14	10	10
2	15	9	9
2	19	9	12
3	0	19	20
3	1	44	43
3	2	37	37
3	3	22	22
3	4	55	55
3	5	6	6
3	6	62	62
3	7	15	15

K	L	FO	FC
3	12	36	36
3	14	24	25
4	0	53	55
4	1	11	11
4	2	27	27
4	3	13	13
4	4	25	26
4	5	28	27
4	6	6	4
4	8	22	21
4	11	10	10
4	13	9	8
4	14	21	23
4	16	13	14
5	0	9	9
5	1	42	43
5	2	21	22
5	3	53	53
5	6	36	36
5	7	31	31
5	9	35	35
5	11	19	19
5	12	14	16
5	13	9	10
5	14	12	12
5	15	15	14
6	0	29	29
6	1	22	22
6	2	44	45
6	3	19	20
6	4	13	12
6	5	57	59
6	7	31	32
6	8	32	33
6	10	16	17
6	11	34	38
6	13	27	27
6	15	9	6
6	16	9	11
7	0	36	36
7	2	9	10
7	3	19	20
7	4	58	60
7	6	59	61
7	8	21	22
7	9	10	11
7	10	28	28
7	12	31	31
7	14	22	22
8	0	21	21
8	1	10	11
8	2	51	52
8	3	12	13
8	4	34	35
8	5	31	32
8	6	11	11

K	L	FO	FC
8	7	19	20
8	8	19	18
9	10	21	21
8	11	12	12
8	13	21	22
9	14	15	15
9	16	15	15
9	0	10	10
9	1	47	48
9	3	41	43
9	4	10	11
9	5	10	11
9	7	27	26
9	9	17	17
9	11	15	15
9	15	22	21
10	0	14	16
10	2	23	22
10	3	10	10
10	4	19	20
10	5	18	18
10	6	21	20
10	8	13	13
10	9	10	10
10	10	16	15
10	11	10	9
10	13	12	14
13	14	16	14
11	3	8	8
11	4	25	25
11	5	3	6
11	6	23	24
11	12	19	19
12	2	12	11
12	3	7	9
12	4	9	11
12	5	22	24
12	7	12	12
12	8	10	11
12	11	17	16
12	13	10	9
13	1	24	25
13	3	26	27
13	4	11	11
13	6	11	10
13	7	15	14
13	9	21	20
14	0	17	17
14	1	11	9
14	2	23	23
14	3	12	11
14	4	15	14
14	5	12	12
14	7	9	7
14	8	15	15
14	10	10	7

K	L	FO	FC
14	11	10	8
15	0	19	19
15	3	9	8
15	4	23	23
15	6	27	26
15	7	11	10
16	1	10	10
15	5	17	18
16	2	10	8
	M=	4	
0	0	7	7
0	4	66	66
0	6	28	28
0	10	24	25
0	12	39	39
1	0	33	33
1	2	26	26
1	3	9	8
1	4	14	14
1	5	45	45
1	6	29	30
1	8	12	13
1	9	12	12
1	10	23	23
1	11	29	29
1	13	15	15
1	14	16	15
2	1	49	49
2	2	7	7
2	3	36	35
2	4	9	9
2	5	10	12
2	7	31	31
2	9	23	24
2	10	14	14
2	11	10	8
2	13	15	16
2	15	14	16
3	0	28	27
3	2	45	46
3	3	25	25
3	4	8	6
3	6	10	9
3	9	17	16
3	9	12	12
3	11	11	11
3	12	9	9
3	13	9	10
3	14	14	14
4	0	10	11
4	2	31	32
4	3	7	5
4	4	26	26
4	5	16	16

K	L	FO	FC
4	6	24	25
4	8	14	14
4	10	25	26
4	12	19	20
4	16	9	10
5	0	14	14
5	2	24	25
5	3	35	36
5	4	20	19
5	5	25	26
5	6	7	6
5	8	16	17
5	9	19	19
5	11	23	24
5	13	14	15
5	15	6	6
6	1	32	31
6	2	16	16
6	3	39	39
6	4	15	15
6	6	14	13
6	7	23	24
6	8	8	7
6	9	26	26
6	10	9	7
6	11	13	15
6	12	12	11
6	16	9	6
7	0	35	35
7	2	42	43
7	3	7	6
7	4	24	25
7	5	16	17
7	6	18	18
7	8	26	27
7	10	17	17
7	11	10	10
7	13	9	8
7	14	21	20
8	0	8	8
8	1	28	29
8	2	11	9
8	3	10	11
8	4	40	40
8	6	16	16
8	7	21	20
8	9	13	15
8	10	15	14
8	12	27	28
8	13	10	11
8	14	10	7
8	15	12	11
9	0	9	10
9	1	10	8
9	2	11	10
9	3	16	16

K	L	FO	FC
9	4	8	7
9	5	29	29
9	9	9	6
9	11	21	21
9	13	16	15
10	1	23	24
10	3	16	16
10	4	24	24
10	7	16	16
10	9	11	10
10	12	11	12
11	0	21	19
11	2	18	19
11	4	9	9
11	6	14	15
11	8	12	13
11	10	11	9
12	0	10	9
12	3	16	16
12	4	8	9
12	6	13	12
12	7	13	13
12	9	10	9
13	3	17	17
13	5	21	21
14	0	10	9
14	1	18	17
14	2	10	10
14	3	14	14
14	4	19	21
14	6	16	15
15	0	19	18
15	2	26	26
15	4	10	11
16	3	9	9
	M=	5	
0	0	39	39
0	2	35	36
0	4	19	19
0	6	30	30
0	8	27	26
0	10	17	16
0	12	12	9
0	14	9	8
1	0	9	9
1	1	23	22
1	2	12	12
1	3	35	36
1	4	29	30
1	5	12	10
1	6	17	17
1	9	18	18

Table A-3. (Continued)

K	L	FO	FC
1	10	13	14
1	12	15	14
2	2	19	19
2	3	23	29
2	4	9	9
2	5	18	19
2	9	10	9
2	10	4	8
2	11	21	21
2	15	3	5
3	0	14	13
3	1	33	31
3	2	12	12
3	4	16	16
3	7	9	9
3	9	11	9
3	10	14	16
3	12	13	13
4	0	32	32
4	2	41	41
4	5	7	8
4	6	9	8
4	8	17	16
4	10	9	9
4	14	12	12
5	1	33	33
5	3	13	11
5	4	7	3
5	5	8	7
5	7	26	26
5	9	19	17
5	12	9	6
6	0	14	14
6	2	12	12
6	3	15	15
6	5	26	26
6	6	11	11
6	9	11	9
6	9	14	14
6	11	14	15
7	0	12	13
7	2	11	10
7	3	11	9
7	4	31	31
7	6	16	16
7	7	9	8
7	8	9	8
7	10	17	17
7	12	17	17
8	0	31	32
8	1	12	12
8	2	26	27
8	3	16	16
8	6	15	15
8	7	9	9
8	8	15	14
8	10	13	13
8	0	9	9
8	2	23	27
8	3	15	17
8	4	14	13
8	7	10	11
8	8	9	4
8	9	16	15
8	10	9	5
9	0	10	11
9	2	12	12
9	3	14	13
9	4	14	17
9	10	11	12
9	3	10	10
9	5	15	15
9	8	10	9
9	1	18	19
9	4	9	7
9	7	15	15
9	8	19	18
9	2	20	19
H= 6			
0	0	11	9
0	2	22	22
0	4	26	26
0	6	13	13
0	10	19	18
0	12	14	12
1	0	22	22
1	3	21	21
1	4	9	8
1	5	16	15
1	6	12	13
1	8	15	13
1	11	15	13
1	12	9	6
2	1	27	26
2	5	17	17
2	7	18	18
2	9	16	15
3	0	27	26
3	1	7	8
3	2	20	20
3	3	12	11
3	6	16	14
3	8	14	14
3	9	10	10
4	1	7	6
4	2	13	11
4	3	10	8
4	4	14	14
4	5	9	8
4	10	12	12
5	1	11	10
5	2	13	14
5	3	19	19
5	5	10	11
5	9	11	10
6	1	21	20
6	2	17	16
6	4	10	10
6	5	15	13
6	7	22	21
6	9	9	11
6	10	9	8
7	0	25	25
7	2	19	19
7	6	16	16
7	8	17	16
8	1	15	14
8	2	12	11
8	3	11	8
8	4	9	10
8	7	9	8
9	1	8	6
9	3	17	17
9	5	10	9
10	1	9	9
10	2	10	8
11	0	12	11
11	6	11	11
12	1	11	10
H= 7			
0	0	13	15
0	4	9	11
0	6	17	16
0	8	11	12
1	1	12	13
1	2	12	11
2	1	11	10
2	3	11	13
3	2	9	8
4	0	15	15
4	6	10	9
5	3	9	7
5	5	14	13
5	7	13	12
6	0	8	6
6	3	14	12
6	5	12	10
7	2	9	11
7	4	9	10
8	0	13	11
9	1	11	11
H= 8			
0	2	13	12
1	3	10	8
4	2	10	8
5	1	10	9

Table A-4. Observed (FO) and Calculated (FC) Structure Factors for $[Cu(\ell\text{-Eph})(\ell\text{-EphH})]_2(ClO_4)_2 \cdot 2H_2O$

K	L	FO	FC
	H=-15		
4	3	14	11
4	4	10	8
4	6	13	10
5	-7	14	12
5	-4	16	14
5	-2	13	11
5	0	12	14
5	1	11	10
5	4	19	10
5	5	13	11
6	-8	16	15
6	-5	17	16
6	-4	12	13
6	-3	16	12
6	-2	19	16
6	-1	12	12
6	0	12	11
6	1	14	17
6	2	15	12
6	4	12	14
6	7	17	12
7	-8	15	12
7	-7	14	10
7	-1	14	13
7	0	13	8
7	1	13	12
7	2	13	16
7	4	12	10
8	2	13	12
8	7	10	8
9	-6	14	14
9	-3	13	14
9	2	10	9
9	3	14	13
9	5	13	10
9	8	11	9
10	-9	20	17
10	-3	14	4
10	-2	16	18
10	1	11	16
10	2	11	11
10	4	13	15
11	-4	15	15
11	-1	15	17
11	2	16	16
11	5	16	13
	H=-14		
2	4	11	9
2	8	10	4
3	-10	13	10
3	-7	13	11
3	0	10	12
3	2	11	15
3	3	11	13
3	6	11	9
3	8	13	11
3	9	12	11
4	-12	14	10
4	-9	15	13
4	-8	13	8
4	-7	14	14
4	-6	14	13
4	-4	18	17
4	-2	12	11
4	-1	18	19
4	0	12	9
4	1	16	15
4	2	15	17
4	4	11	13
4	5	12	14
4	8	12	13
4	10	10	10
4	11	13	12
5	-13	13	14
5	-10	20	18
5	-7	24	24
5	-4	31	32
5	-3	13	14
5	-1	26	27
5	0	12	13
5	2	30	29
5	3	13	9
5	5	28	26
5	8	19	19
5	11	15	16
6	-12	14	12
6	-9	14	16
6	-6	17	17
6	-3	18	18
6	-1	12	9
6	0	14	16
6	1	13	9
6	2	12	10
6	3	14	15
6	4	10	9
6	6	11	11
7	-8	14	14
7	-4	12	13
7	-2	12	11
7	2	12	8
8	-6	12	9
8	3	9	8
8	5	10	9
8	7	11	11
9	-9	15	14
9	-6	17	13
9	-4	16	17
9	-3	12	14
9	-1	18	21
9	0	18	16
9	2	19	23
9	3	14	13
9	5	20	23
9	6	16	12
9	8	14	17
9	11	13	13
10	-9	20	22
10	-6	27	26
10	-3	28	28
10	-1	13	14
10	0	30	29
10	2	13	12
10	3	28	29
10	4	11	4
10	6	23	23
10	9	20	18
10	12	15	13
11	-6	13	11
11	-5	13	15
11	-2	13	14
11	1	12	12
11	3	10	11
11	4	10	10
12	1	10	10
12	3	12	10
12	7	12	7
	H=-13		
0	-4	12	7
0	-1	12	8
0	2	17	14
0	3	13	11
0	8	11	9
1	-4	12	14
1	-1	12	16
1	0	12	10
1	3	11	11
1	9	11	11
2	-12	19	17
2	-9	23	23
2	-6	24	29
2	-3	26	28
2	0	23	27
2	1	10	9
2	3	31	31
2	6	28	27
2	7	10	7
2	9	23	23
2	10	11	6
2	12	20	18
3	-11	14	13
3	-8	16	16
3	-5	19	16
3	-2	15	16
3	1	17	21
3	2	13	8
3	3	11	12
3	4	23	21
3	6	15	14
3	7	13	11
3	9	10	11
4	-3	12	14
4	-1	13	12
4	0	20	17
4	6	10	8
4	9	11	7
5	-2	13	10
5	3	10	7
5	5	13	12
5	7	12	11
5	8	10	12
5	10	10	10
5	11	10	11
6	-5	17	18
6	-8	18	16
6	-6	17	21
6	-5	15	15
6	-2	17	11
6	-1	12	10
6	0	12	17
6	1	16	12
6	2	11	10
6	3	20	20
6	4	9	7
6	6	20	21
6	9	16	19
6	12	20	18
6	15	15	12
7	-11	18	20
7	-8	18	21
7	-6	16	13
7	-5	24	29
7	-3	12	11
7	-2	26	28
7	-1	11	7
7	1	18	25
7	4	20	24
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Table A-4. (Continued)

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Table A-4. (Continued)

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Table A-4. (Continued)

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11	-7	30	30	14	-1	13	9	1	-3	59	53	3	-16	11	8	4	2	68	63	6	-14	26	24	7	12	34	33	9	11	12	13
11	-6	15	15	14	0	16	16	1	-2	20	22	3	-15	26	26	4	3	49	46	6	-12	28	33	7	13	24	22	9	12	22	20
11	-5	21	19	14	1	11	10	1	-1	48	47	3	-14	25	24	4	4	40	38	6	-11	29	26	7	14	10	6	9	14	10	10
11	-4	35	35	14	3	17	17	1	0	47	49	3	-13	13	11	4	5	61	59	6	-10	16	12	7	15	23	24	9	15	19	17
11	-3	23	22	14	4	13	10	1	1	29	28	3	-12	34	37	4	6	33	34	6	-9	35	38	7	16	11	9	9	18	12	15
11	-2	25	26	14	5	11	9	1	2	24	22	3	-11	34	35	4	7	38	36	6	-8	39	36	7	17	13	12	10	-10	12	12
11	-1	43	41	14	6	16	17	1	3	28	32	3	-10	27	25	4	8	46	50	6	-7	31	28	7	19	9	4	10	-15	17	16
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11	1	34	34	15	1	13	13	1	5	25	27	3	-8	35	36	4	10	32	36	6	-5	34	37	8	-17	11	10	10	-12	11	11
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11	3	29	29	15	5	11	10	1	7	19	17	3	-6	56	56	4	12	25	24	6	-3	69	65	8	-13	35	38	10	-9	19	28
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11	5	34	34					1	9	12	20	3	-4	49	49	4	14	46	45	6	-1	36	36	8	-11	11	3	10	-7	18	12
11	6	23	22		H=	-7		1	10	21	22	3	-3	78	78	4	15	18	19	6	0	51	47	8	-10	56	60	10	-6	26	27
11	7	13	12					1	11	18	17	3	-2	50	57	4	16	20	22	6	1	44	44	8	-9	23	24	10	-5	31	31
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11	9	23	21	0	-16	20	23	1	14	16	15	3	0	50	49	4	18	10	9	6	3	39	38	8	-7	68	66	10	-3	13	21
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12	15	13	6	1	-11	18	20	2	16	12	7	4	-5	58	58	5	12	23	22	7	4	44	45	9	3	47	44	11	3	14	18
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13	-7	13	11	1	-9	53	52	2	19	10	7	4	-3	62	50	5	14	19	19	7	6	60	63	9	5	19	17	11	5	16	15
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Table A-4. (Continued)

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11	18	10	9
11	19	10	8
12	-16	12	10
12	-13	14	16
12	-10	19	17
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12	13	13	10
12	14	10	7
13	-15	14	12
13	-12	15	17
13	-9	15	19
13	-6	19	20
13	-3	16	19
13	-1	15	12
13	0	13	10
13	1	9	10
13	2	15	12
13	5	17	19
13	6	19	21
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14	4	11	13
14	5	10	10
14	8	13	14
14	12	10	6
15	-4	13	11
15	-2	13	12
15	2	12	9
15	7	11	9

M= 6

K	L	FC	FC
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0	-16	17	16
0	-14	34	37
0	-13	14	14
0	-12	17	10
0	-11	39	44
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1	-17	15	19
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1	-9	14	13
1	-8	26	25
1	-7	22	26
1	-5	43	43
1	-4	34	34
1	-3	36	34
1	-2	60	57
1	-1	65	79
1	0	47	48
1	1	35	30
1	2	66	63
1	3	59	55
1	4	47	49
1	5	37	35
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1	7	26	26
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1	9	47	45
1	10	24	21
1	12	38	42
1	13	20	24
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1	16	27	25
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1	21	12	11
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2	3	66	62
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2	6	59	53
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2	9	46	47
2	10	42	43
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2	12	41	42
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3	-2	71	62
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3	4	78	74
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6	11	39	42
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7	0	47	49
7	1	47	45
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7	13	15	10
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8	4	88	90
8	5	23	22
8	6	16	15
8	7	88	81
8	8	11	7
8	9	13	14
8	10	61	61
8	11	12	9
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8	16	22	21
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12	15	11	11
12	16	11	9
12	-16	14	13
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13	-4	19	23
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13	2	24	29

Table A-4. (Continued)

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15	-5	12	10
15	-7	12	7
15	-6	13	10
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0	-12	25	24
0	-11	55	56
0	-10	41	38
0	-9	19	17
0	-8	54	58
0	-7	24	23
0	-6	87	95
0	-5	102	116
0	-4	19	18
0	-3	85	76
0	-2	80	92
0	0	74	68
0	1	97	96
0	2	18	18
0	3	56	52
0	4	121	129
0	5	19	17
0	6	55	58
0	7	85	94
0	8	29	33
0	9	21	24
0	10	63	63
0	11	23	25
0	13	49	48
0	14	14	19
0	15	41	39
0	19	25	21
0	22	13	15
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1	-18	13	11

K	L	FO	FC
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1	-14	22	25
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1	1	46	43
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1	4	62	54
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1	18	20	18
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2	-4	15	10
2	-3	53	51
2	-2	36	27
2	-1	28	31
2	0	60	53
2	1	20	23
2	2	45	36
2	3	46	57

K	L	FO	FC
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2	5	51	48
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2	7	28	30
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K	L	FO	FC
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4	-7	38	39
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4	-4	19	8
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4	9	49	45
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4	13	25	24
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5	-9	19	23
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5	3	83	76
5	4	17	19
5	5	107	116
5	6	87	84
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5	8	58	58

K	L	FO	FC
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5	13	21	22
5	14	47	42
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5	16	12	14
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6	-8	13	16
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6	1	66	80
6	2	61	55
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7	-16	11	8
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7	-13	29	29
7	-11	25	27
7	-10	51	48
7	-9	19	19
7	-8	18	20

K	L	FO	FC
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7	-5	26	29
7	-4	74	77
7	-3	26	24
7	-2	67	65
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7	0	27	25
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7	2	67	61
7	3	42	43
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8	-2	34	29
8	-1	22	16
8	0	56	58
8	1	27	28
8	2	26	24
8	3	51	52
8	4	55	53
8	5	16	14
8	6	36	34
8	7	31	31
8	8	12	15
8	9	46	47
8	10	15	16
8	11	9	13
8	12	30	31
8	13	24	23
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8	16	15	16
8	19	14	15
8	22	12	9

K	L	FC	FC
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9	0	30	30
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9	10	25	28
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10	-5	17	20
10	-4	29	28
10	-3	34	38
10	-2	20	22
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10	1	33	31
10	2	35	33
10	3	39	39
10	4	29	30
10	5	15	13
10	6	42	38
10	7	35	37
10	9	36	36

K	L	FO	FC
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10	12	24	25
10	13	19	16
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10	15	15	14
10	16	12	8
10	18	11	8
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Table A-4. (Continued)

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0	-15	25	29
0	-14	13	12
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0	-9	46	48
0	-8	36	30
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0	-5	67	64
0	-4	65	59
0	-3	54	50
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0	1	26	25
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2	-8	43	50
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2	-1	61	65
2	0	47	60
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2	2	10	14
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2	4	59	62
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12	-3	17	17
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12	2	11	9
12	3	15	20
12	6	15	16
12	7	13	16
12	10	19	20
12	13	13	13
13	-4	14	9
13	-3	14	14

Table A-4. (Continued)

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14	-8	23	23
14	-3	25	25
14	0	31	25
14	1	14	13
14	3	32	27
14	8	23	26
14	9	23	21
14	12	13	12
15	-5	13	13
15	-2	14	16
15	1	12	17
15	4	15	19

H= -3

K	L	FO	FC
0	-17	11	12
0	-14	23	36
0	-13	13	16
0	-12	14	13
0	-11	23	18
0	-10	41	44
0	-9	33	30
0	-8	24	33
0	-7	59	49
0	-6	52	51
0	-5	77	62
0	-4	36	19
0	-3	13	24
0	-2	55	62
0	-1	113	90
0	0	56	50
0	1	93	68
0	2	56	57
0	3	63	54
0	4	89	78
0	5	63	67
0	6	42	36
0	7	23	36
0	8	73	67
0	9	32	37
0	10	19	30
0	11	67	62
0	12	21	29
0	13	11	12
0	14	42	41
0	16	16	27
0	17	22	26
0	20	19	23
0	23	16	17
1	-22	13	7
1	-20	10	16

K	L	FO	FC
1	-19	19	15
1	-17	23	22
1	-16	30	29
1	-15	14	10
1	-14	22	36
1	-13	42	43
1	-12	34	33
1	-11	68	74
1	-10	49	56
1	-9	26	27
1	-8	83	70
1	-7	60	61
1	-6	44	41
1	-5	141	123
1	-4	70	82
1	-3	54	55
1	-2	162	157
1	-1	76	75
1	0	142	128
1	1	43	35
1	2	85	99
1	3	88	88
1	4	55	41
1	5	141	133
1	6	84	75
1	7	36	42
1	8	76	78
1	9	52	58
1	10	12	9
1	11	36	36
1	12	42	43
1	13	27	29
1	14	34	39
1	15	37	43
1	17	13	22
1	18	27	31
1	21	13	20
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2	-23	11	7
2	-20	21	22
2	-19	12	16
2	-17	34	31
2	-15	12	10
2	-14	42	43
2	-12	38	32
2	-11	120	122
2	-10	12	31
2	-9	39	45
2	-8	151	147
2	-7	26	29
2	-6	20	24
2	-5	84	75
2	-4	49	47
2	-3	29	28
2	-2	187	173
2	-1	32	47

K	L	FO	FC
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2	1	185	177
2	2	44	34
2	3	149	134
2	4	41	35
2	5	174	154
2	6	87	73
2	7	90	86
2	8	18	20
2	9	23	24
2	10	56	63
2	11	19	21
2	12	33	34
2	13	53	57
2	14	26	20
2	15	18	19
2	16	46	43
2	19	34	36
3	-26	12	7
3	-23	11	16
3	-20	18	21
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3	7	62	53
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4	3	46	44
4	4	52	47
4	5	63	60
4	6	46	44
4	7	52	60
4	8	18	9
4	9	65	65
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5	-14	18	22
5	-13	10	9
5	-12	11	16
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6	1	21	25
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7	-17	26	27
7	-16	19	24
7	-15	18	18
7	-14	42	44

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7	-11	43	41
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8	-7	36	38
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8	2	41	41
8	3	12	15
8	4	11	5
8	5	34	31
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8	8	30	30
8	11	20	23
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K	L	FO	FC
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11	-17	13	14
11	-14	16	16
11	-11	25	25
11	-8	40	38
11	-5	42	42
11	-2	41	49
11	-1	12	6

K	L	FO	FC
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11	1	53	54
11	3	27	24
11	4	41	42
11	6	19	22
11	7	36	35
11	9	15	19
11	10	31	33
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13	-2	12	10
13	0	16	16
13	3	12	12
13	8	13	7
14	-1	15	12
14	6	13	14

H= -2

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0	-19	14	12
0	-18	9	3
0	-17	12	22
0	-16	33	37
0	-15	23	25
0	-14	24	26
0	-13	48	51
0	-11	29	27
0	-10	60	64
0	-9	28	28
0	-8	65	78
0	-7	77	95
0	-6	63	53
0	-5	52	67
0	-4	151	139
0	-3	152	148
0	-2	45	18

Table A-4. (Continued)

K	L	FC	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC
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0	0	57	60	2	-8	23	24	3	10	51	57	5	-12	14	20	6	10	15	13	8	-4	45	53	10	-5	18	14	13	4	14	13
0	1	171	161	2	-7	29	31	3	11	67	72	5	-11	19	21	6	11	53	51	8	-3	36	33	10	-4	36	37	13	7	13	14
0	2	93	91	2	-6	48	59	3	12	35	36	5	-10	28	28	6	12	32	33	8	-2	60	63	10	-3	11	9	13	9	12	7
0	3	162	154	2	-5	67	66	3	13	42	46	5	-9	26	33	6	13	18	18	8	-1	52	56	10	-1	43	44	13	11	13	11
0	4	123	120	2	-4	118	116	3	14	22	34	5	-8	41	42	6	14	30	29	8	0	17	19	10	2	25	31	14	-1	13	10
0	5	67	64	2	-3	162	156	3	16	31	31	5	-7	14	17	6	15	12	12	8	1	67	73	10	3	21	16	14	0	12	10
0	6	43	57	2	-2	92	75	3	17	20	21	5	-6	47	38	6	16	12	12	8	2	95	66	10	5	11	16				
0	7	29	32	2	-1	173	164	3	19	19	15	5	-5	64	62	6	17	16	18	8	3	18	19	10	6	34	34		H= -1		
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1	5	75	73	3	-10	18	13	4	9	62	58	6	-10	33	35	7	12	36	37	9	2	42	46	12	0	12	14	1	-16	13	11
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1	13	33	51	3	-2	97	103	4	17	14	27	6	-2	80	83	8	-17	16	13	9	11	24	22	12	13	12	14	1	-7	87	103
1	14	25	19	3	-1	38	29	4	18	12	16	6	-1	76	72	8	-16	19	15	9	13	16	15	12	14	13	9	1	-6	40	59
1	15	15	36	3	0	149	134	4	19	22	21	6	0	21	26	8	-14	12	13	9	14	15	19	13	-10	14	14	1	-5	123	143
1	16	23	30	3	1	73	71	4	22	12	11	6	1	54	51	8	-13	25	29	9	16	11	8	13	-7	16	16	1	-4	146	170
1	18	15	12	3	2	158	151	5	-21	14	15	6	2	67	74	8	-12	21	26	9	17	15	18	13	-6	13	13	1	-3	170	179
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2	-12	44	41	3	7	63	53	5	-15	21	27	6	7	32	31	8	-7	52	55	10	-10	17	18	13	0	15	14	1	5	229	226
2	-10	33	42	3	8	81	70	5	-14	28	31	6	8	66	68	8	-6	16	21	10	-9	12	13	13	1	11	12	1	6	69	66

Table A-4. (Continued)

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2	-12	45	44
2	-11	26	29
2	-10	41	46
2	-9	61	47
2	-8	45	53
2	-7	53	47
2	-6	23	23
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2	-4	174	169
2	-3	29	40
2	-2	20	25
2	-1	73	75
2	0	73	68
2	1	65	63
2	2	52	49
2	3	142	128
2	4	141	129
2	5	77	97
2	6	156	161
2	7	43	52
2	8	77	99
2	9	63	68
2	10	63	64
2	11	43	44
2	12	17	14
2	13	30	39
2	14	31	26
2	15	25	25
2	19	15	19
3	-22	11	9
3	-21	11	15
3	-19	33	36
3	-18	12	11
3	-17	12	12
3	-16	44	42
3	-15	21	20
3	-14	26	19
3	-13	49	54
3	-12	33	35
3	-11	19	18
3	-10	51	61
3	-9	22	26
3	-8	16	17
3	-7	27	28
3	-6	92	71
3	-5	173	157
3	-4	32	25
3	-3	141	129
3	-2	33	29
3	-1	184	178
3	0	149	126
3	1	33	48
3	2	200	173
3	3	24	24
3	4	54	50
3	5	82	73
3	6	19	20
3	7	25	26
3	9	151	147
3	9	44	48
3	11	121	124
3	12	39	31
3	14	42	44
3	15	13	8
3	17	33	31
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4	-11	48	54
4	-10	49	49
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4	-8	75	70
4	-7	37	37
4	-6	70	79
4	-5	67	58
4	-4	30	32
4	-3	81	87
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4	-1	91	76
4	0	25	25
4	1	99	100
4	2	40	42
4	3	101	79
4	4	47	42
4	5	29	32
4	6	42	33
4	7	45	48
4	8	73	65
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5	-10	65	63
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5	-8	11	15
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5	-5	55	45
5	-4	63	63
5	-3	25	26
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5	3	28	24
5	4	22	8
5	5	75	63
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5	8	63	62
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5	10	27	27
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5	12	19	22
5	13	17	17
5	14	14	16
5	16	15	11
5	19	10	8
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6	-15	10	7
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6	-11	26	30
6	-10	17	16
6	-9	27	22
6	-8	17	18
6	-7	12	11
6	-6	27	24
6	-5	19	23
6	-4	53	56
6	-3	19	16
6	-2	45	42
6	-1	34	36
6	0	72	69
6	1	39	41
6	2	29	36
6	3	46	38
6	4	53	51
6	6	19	27
6	7	14	15
6	8	18	19
6	9	19	20
6	10	23	25
6	11	14	12
6	12	22	20
6	13	29	29
6	14	12	15
6	15	25	25
6	16	23	21
6	18	12	14
6	19	18	10
6	21	15	11
6	22	13	10
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7	-13	17	20
7	-12	28	32
7	-11	21	25
7	-10	32	36
7	-9	36	39
7	-8	33	32
7	-7	24	24
7	-6	42	42
7	-5	44	47
7	-4	43	42
7	-3	38	38
7	-2	55	52
7	-1	46	43
7	0	52	48
7	1	36	38
7	2	22	28
7	3	69	64
7	4	29	33
7	5	34	38
7	6	42	41
7	7	29	29
7	8	36	35
7	9	35	36
7	10	13	12
7	11	28	27
7	12	29	33
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8	-6	52	53
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8	-3	56	58
8	-2	33	35
8	-1	34	34
8	0	62	62
8	1	57	60
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8	5	24	24
8	6	58	62
8	7	29	33
8	8	16	27
8	9	50	47
8	10	32	30
8	11	19	20
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8	13	10	8
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8	15	21	21
8	16	14	12
8	18	17	17
8	21	14	12
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9	-10	12	19
9	-9	14	19
9	-8	10	9
9	-7	15	14
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9	-5	19	22
9	-4	30	27
9	-3	23	27
9	-2	21	22
9	-1	21	21
9	0	15	21
9	2	15	22
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9	8	23	20
9	9	12	12
9	12	12	17
9	14	10	11
9	16	11	12
10	-15	12	9
10	-12	21	20
10	-11	17	12
10	-10	11	13
10	-9	19	17
10	-8	17	18
10	-7	26	27
10	-6	16	19
10	-5	27	26
10	-4	25	24
10	-3	30	36
10	-2	35	31
10	-1	18	18
10	0	26	28
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10	2	27	25
10	3	22	21
10	4	25	21
10	5	20	21
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11	-2	12	15
11	1	17	15
11	8	20	19
11	11	14	14
11	12	11	2
11	14	13	14
11	17	12	11
12	-10	20	18
12	-8	13	11
12	-7	23	24
12	-4	22	25
12	-1	27	27
12	2	25	25
12	4	14	8
12	5	19	20
12	8	20	21
12	11	17	16
13	-3	14	12
13	-6	13	14
13	-5	12	14
13	-4	12	12
13	-2	17	15
13	1	17	18
13	4	16	17
13	7	13	13
H= 0			
0	6	189	169
0	9	164	173
0	12	50	56
0	15	18	18
0	18	53	50
0	21	13	10
1	2	81	94
1	3	169	180
1	4	150	171
1	5	129	144
1	6	42	62
1	7	89	105
1	8	37	27
1	9	47	35
1	10	52	44
1	11	21	19
1	12	15	30
1	16	11	12
2	0	67	68
2	1	170	161
2	2	91	81
2	3	161	154
2	4	122	119
2	5	66	64
2	6	48	57
2	7	29	31
2	8	22	24
2	9	62	61
2	10	40	42
2	12	41	40
2	13	20	27
2	15	26	30
2	16	11	15
2	19	12	10
3	0	58	50
3	1	82	69
3	2	86	97
3	3	65	54
3	4	88	77
3	5	63	67
3	6	43	38
3	7	28	35
3	8	78	68
3	9	32	36
3	11	67	63
3	12	25	31
3	14	42	41
3	16	17	27
3	17	25	26
3	20	19	23
3	23	16	17
4	0	30	28
4	1	27	25
4	2	69	57
4	3	74	67
4	4	53	43
4	5	69	67
4	6	69	68
4	7	20	22
4	8	57	51
4	9	62	66
4	10	11	12
4	11	32	29
4	12	41	43
4	13	15	18
4	14	26	28
4	15	26	30
4	16	15	17
4	17	17	18
4	18	19	17
4	21	15	14
5	0	76	69
5	1	98	96
5	2	16	17
5	3	54	52
5	4	122	129
5	5	20	17
5	6	54	59
5	7	85	83
5	8	27	33
5	9	20	25
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5	19	22	22
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6	1	30	28
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6	7	16	20
6	8	23	23
6	10	17	20
6	12	21	19
6	13	18	18
6	15	15	8
6	17	11	12
7	0	29	32
7	1	23	28
7	2	35	38
7	3	41	42
7	4	42	44
7	5	49	50
7	6	41	39
7	7	27	31
7	8	35	37

Table A-4. (Continued)

K	L	FC	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC
7	9	23	25												
7	10	13	16												
7	11	22	22												
7	12	14	17												
7	13	14	16												
7	14	13	16												
7	17	13	11												
8	0	24	23												
8	2	13	13												
8	3	45	47												
8	5	11	7												
8	6	42	44												
8	8	12	10												
8	9	30	28												
8	10	14	11												
8	12	17	18												
8	15	17	17												
9	0	42	43												
9	1	13	21												
9	2	27	31												
9	3	31	32												
9	4	23	21												
9	5	15	17												
9	6	26	26												
9	7	16	12												
9	8	12	12												
9	9	20	20												
9	10	17	21												
9	13	24	21												
9	14	15	13												
9	21	14	7												
10	0	15	19												
10	1	16	11												
10	2	31	33												
10	3	12	17												
10	5	22	25												
10	6	17	16												
10	7	27	27												
10	9	23	17												
10	11	21	21												
10	12	15	16												
11	8	15	14												
11	9	12	8												
12	0	14	13												
12	1	13	18												
12	3	13	15												
12	4	23	20												
12	7	14	19												
12	10	13	15												
13	2	13	14												

Table A-5. Observed (FO) and Calculated (FC) Structure Factors for $[Co_2(Deta)_2(DetaH)_2]_2(ClO_4)_2$

K	L	FO	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
	H=	0		2	8	22	21	4	11	28	26	7	-6	49	47	9	6	57	57	12	10	16	18	16	-3	13	15	0	12	77	73
				2	9	20	20	4	12	23	23	7	-5	49	49	9	7	29	28	12	11	57	58	16	-2	31	31	0	14	20	21
0	-12	11	12	2	10	43	44	4	13	26	26	7	-4	111	104	9	8	25	24	12	12	15	14	16	-1	12	11	1	-15	27	29
0	-10	41	34	2	11	11	14	4	14	13	9	7	-3	104	98	9	10	28	28	13	-11	19	16	16	0	19	18	1	-14	18	19
0	-8	63	64	2	12	36	35	5	-14	51	51	7	-2	31	34	9	12	33	41	13	-10	19	18	16	1	13	11	1	-12	15	14
0	-6	53	53	2	13	32	31	5	-13	10	5	7	-1	52	50	10	-12	10	9	13	-7	54	55	16	2	31	31	1	-11	88	92
0	-2	9	9	2	15	34	33	5	-12	28	29	7	1	51	50	10	-11	68	67	13	-6	41	40	16	3	15	15	1	-10	10	9
0	2	10	9	3	-14	38	38	5	-9	18	20	7	2	31	34	10	-9	26	26	13	-5	11	13	16	4	38	37	1	-9	41	43
0	4	53	53	3	-12	26	27	5	-8	60	59	7	3	105	98	10	-7	56	56	13	-4	28	27	16	6	17	21	1	-8	16	13
0	8	63	64	3	-11	34	36	5	-7	57	55	7	4	109	104	10	-6	25	24	13	-3	48	50	16	8	29	27	1	-7	28	28
0	10	33	34	3	-10	35	35	5	-6	35	35	7	5	50	49	10	-5	20	19	13	-2	19	18	16	9	27	26	1	-6	44	44
0	12	12	12	3	-9	16	16	5	-5	31	30	7	6	48	47	10	-4	24	25	13	2	16	18	17	-8	20	18	1	-5	31	30
1	-14	13	6	3	-8	72	73	5	-4	108	109	7	7	49	50	10	-2	38	38	13	3	44	50	17	-7	24	25	1	-4	44	43
1	-13	15	13	3	-7	61	62	5	-3	87	84	7	8	37	37	10	-1	52	52	13	4	27	27	17	-5	20	19	1	-1	89	86
1	-10	19	18	3	-6	16	17	5	-2	63	63	7	10	9	9	10	0	58	58	13	5	13	13	17	-4	12	16	1	-1	231	222
1	-9	32	34	3	-5	101	97	5	-1	61	62	7	11	9	12	10	1	51	52	13	6	40	40	17	-3	33	34	1	0	8	5
1	-8	3	9	3	-3	50	48	5	1	61	62	7	13	12	12	10	2	39	38	13	7	55	55	17	-2	13	11	1	1	39	35
1	-7	12	12	3	-2	63	64	5	2	62	63	7	14	35	34	10	3	3	5	13	9	10	7	17	-1	20	21	1	2	115	113
1	-6	25	27	3	-1	109	100	5	3	87	84	8	-13	21	19	10	4	25	25	13	10	13	18	17	1	22	21	1	3	45	43
1	-5	76	75	3	1	104	100	5	4	109	109	8	-12	11	12	10	5	13	13	13	11	14	16	17	3	35	34	1	4	69	72
1	-4	13	10	3	2	65	64	5	5	30	30	8	-11	44	44	10	6	26	24	14	-11	28	29	17	4	16	16	1	5	68	68
1	-3	38	37	3	3	51	48	5	6	35	35	8	-9	25	24	10	7	56	56	14	-10	10	12	17	5	19	19	1	6	33	32
1	-2	37	29	3	5	100	97	5	7	55	55	8	-8	26	25	10	9	28	26	14	-8	19	20	17	7	25	25	1	7	85	84
1	2	37	28	3	6	16	17	5	8	60	59	8	-7	65	65	10	11	67	67	14	-7	27	26	17	8	20	18	1	9	29	10
1	3	33	37	3	7	59	62	5	9	18	20	8	-6	24	22	10	13	10	4	14	-6	14	14	18	-7	21	20	1	11	20	22
1	4	14	10	3	8	72	73	5	12	30	29	8	-5	7	10	11	-12	41	41	14	-4	37	38	18	-5	10	7	1	13	17	17
1	5	75	75	3	9	17	16	5	14	50	51	8	-4	66	63	11	-10	43	49	14	-3	48	47	18	-2	22	20	1	14	10	14
1	6	26	27	3	10	34	35	6	-14	15	12	8	-3	106	105	11	-8	18	20	14	-2	55	56	18	0	16	13	2	-15	18	18
1	7	12	12	3	11	36	36	6	-13	28	27	8	-2	43	42	11	-7	18	20	14	-1	19	18	18	2	20	20	2	-13	11	11
1	9	34	34	3	12	27	27	6	-12	20	19	8	0	103	99	11	-6	53	54	14	0	11	10	18	7	21	20	2	-12	12	11
1	13	20	18	3	14	38	38	6	-10	21	20	8	2	42	42	11	-5	43	44	14	1	20	18	19	-5	24	25	2	-11	11	9
1	13	16	13	4	-14	12	9	6	-9	71	69	8	3	107	105	11	-4	20	18	14	2	56	56	19	-4	11	10	2	-10	81	82
1	14	11	6	4	-13	24	26	6	-8	57	57	8	4	65	63	11	-1	8	11	14	3	47	47	19	-3	20	19	2	-9	63	65
1	15	11	6	4	-12	21	23	6	-6	33	34	8	5	9	10	11	1	8	11	14	4	37	38	19	-1	24	22	2	-8	20	21
2	-15	35	33	4	-11	28	26	6	-4	95	94	8	6	24	22	11	4	20	18	14	6	11	14	19	1	21	22	2	-7	46	47
2	-13	32	31	4	-10	20	18	6	-3	97	94	8	7	66	65	11	5	44	44	14	7	27	26	19	3	20	19	2	-6	45	43
2	-12	36	35	4	-9	98	96	6	-2	130	127	8	8	25	25	11	6	56	54	14	8	19	20	19	5	26	25	2	-5	10	12
2	-11	16	14	4	-8	44	44	6	-1	120	116	8	9	27	24	11	7	19	20	14	10	12	12	20	-2	15	12	2	-4	37	38
2	-10	43	44	4	-7	31	32	6	0	34	33	8	11	45	44	11	8	17	20	14	11	30	29	20	0	33	32	2	-3	156	147
2	-9	19	20	4	-6	67	68	6	1	118	116	8	12	13	12	11	10	50	49	15	-8	19	18	20	2	15	12	2	-2	37	35
2	-8	22	21	4	-5	14	15	6	2	126	127	8	13	19	19	11	12	42	41	15	-7	37	38	20	4	22	21	2	-1	200	191
2	-7	8	6	4	-4	97	97	6	3	100	94	9	-12	42	41	12	-12	15	14	15	-6	28	27					2	0	205	189
2	-6	83	83	4	-3	93	92	6	4	94	94	9	-10	26	28	12	-11	53	52	15	-5	64	64		H=	1		2	1	76	72
2	-5	40	40	4	-2	85	90	6	6	32	34	9	-8	26	24	12	-10	17	18	15	-2	11	13					2	2	23	25
2	-4	53	57	4	-1	69	64	6	7	7	3	9	-7	29	28	12	-9	21	22	15	-1	21	21	0	-14	27	27	2	3	52	48
2	-3	155	148	4	0	9	6	6	8	58	57	9	-6	56	57	12	-7	42	42	15	1	23	21	0	-10	65	64	2	4	91	89
2	-2	110	110	4	1	68	64	6	9	88	89	9	-5	40	39	12	-6	17	18	15	2	12	13	0	-8	57	55	2	5	45	43
2	-1	10	7	4	2	94	90	6	10	22	20	9	-4	49	48	12	-2	34	34	15	3	65	64	0	-6	106	118	2	6	31	31
2	0	220	209	4	3	43	42	6	12	21	19	9	-3	91	91	12	-1	67	65	15	6	27	27	0	-4	62	66	2	7	36	37
2	1	10	7	4	4	36	37	6	13	27	27	9	-2	63	63	12	0	26	25	15	7	37	38	0	-2	38	33	2	8	38	38
2	2	112	110	4	5	15	15	6	14	14	12	9	-1	49	49	12	1	65	65	15	8	18	18	0	0	168	169	2	9	42	41
2	3	155	148	4	6	67	68	7	-14	36	34	9	1	50	49	12	2	34	34	16	-9	27	26	0	2	238	231	2	10	21	24
2	4	53	57	4	7	31	32	7	-13	12	12	9	2	63	63	12	3	8	6	16	-8	29	27	0	4	60	57	2	11	28	29
2	5	41	40	4	8	44	44	7	-11	10	12	9	3	89	91	12	5	16	18	16	-6	21	21	0	6	45	45	2	12	35	35
2	6	62	63	4	9	95	96	7	-8	37	37	9	4	48	48	12	7	41	42	16	-5	9	1	0	8	8	10	3	-15	29	30
2	7	8	6	4	10	20	18	7	-7	49	50	9	5	41	39	12	9	22	22	16	-4	37	37	0	10	33	34	3	-14	36	35

Table A-5. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
3	-13	21	20	5	-10	37	36	7	-7	91	92	9	0	56	55	12	0	48	41	15	4	14	18	0	-2	27	16	2	11	25	23
3	-12	11	11	5	-9	19	19	7	-6	52	52	9	1	26	29	12	1	43	43	15	5	10	6	0	0	42	41	2	12	45	46
3	-11	37	36	5	-8	28	28	7	-5	55	53	9	2	7	4	12	2	9	10	15	6	12	11	0	2	85	87	3	-15	14	13
3	-10	37	34	5	-7	47	47	7	-4	95	89	9	3	14	12	12	3	12	10	15	7	19	21	0	4	23	26	3	-13	29	29
3	-9	22	24	5	-6	33	30	7	-3	95	94	9	4	10	10	12	4	10	10	15	9	14	21	0	6	137	136	3	-12	47	47
3	-7	28	29	5	-5	29	28	7	-2	53	52	9	6	33	33	12	5	31	32	16	-10	12	1	0	8	47	44	3	-11	75	77
3	-6	24	27	5	-4	54	54	7	1	49	47	9	7	14	13	12	6	28	31	16	-9	22	21	0	12	47	48	3	-8	43	39
3	-5	56	57	5	-3	20	18	7	2	31	30	9	9	32	32	12	7	43	43	16	-8	45	44	1	-15	41	39	3	-7	13	11
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3	1	31	69	5	2	8	6	7	7	36	36	10	-8	20	20	13	-7	41	42	16	2	33	32	1	-9	23	21	3	-2	51	50
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3	12	19	19	5	13	10	11	8	-10	14	15	10	4	25	26	13	4	24	25	17	4	16	16	1	1	62	60	3	9	16	18
3	13	16	17	6	-14	14	12	8	-9	47	48	10	5	41	41	13	5	11	9	17	5	14	14	1	2	19	13	3	10	23	23
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4	-11	20	24	6	-8	98	93	8	-4	85	83	10	11	55	56	14	-11	22	22	18	-1	15	16	1	7	113	115	4	-11	39	37
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4	-1	23	21	6	2	159	155	8	9	25	25	11	2	79	79	14	2	23	22	19	-2	18	21	2	-9	34	34	4	-1	141	140
4	0	124	122	6	3	181	178	8	10	29	29	11	4	61	61	14	4	12	12	19	-1	23	19	2	-8	8	13	4	0	14	12
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4	6	53	59	6	9	14	15	9	-12	28	28	12	-11	35	34	15	-7	46	45	20	-1	21	22	2	0	73	70	4	7	35	36
4	7	61	61	6	10	39	41	9	-11	44	45	12	-10	20	19	15	-6	23	26	20	0	33	32	2	1	53	51	4	8	26	24
4	8	56	55	6	11	13	12	9	-9	21	23	12	-9	21	21	15	-5	10	11	20	2	17	16	2	2	81	84	4	10	31	31
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5	-13	21	23	7	-10	9	7	9	-3	22	21	12	-3	45	45	15	1	20	20	0	-8	53	54	2	8	9	13	5	-9	29	30
5	-12	18	17	7	-9	13	12	9	-2	14	15	12	-2	31	32	15	2	16	15	0	-6	46	48	2	9	9	7	5	-8	84	86
5	-11	11	14	7	-8	19	15	9	-1	39	40	12	-1	19	20	15	3	16	17	0	-4	117	119	2	10	10	7	5	-7	40	38

Table A-5. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
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5	-7	27	26	7	4	22	20	9	10	29	30	12	8	20	19	16	8	17	13	1	-12	13	13	3	0	10	8	5	9	16	17
5	-6	66	65	7	5	40	41	9	11	19	15	12	10	16	13	17	-9	24	28	1	-11	81	84	3	1	76	81	5	10	33	35
5	-5	7	5	7	6	26	26	9	12	22	20	13	-12	15	14	17	-8	27	26	1	-9	50	50	3	3	21	19	5	11	14	13
5	-4	79	76	7	7	33	32	10	-13	11	11	13	-11	10	10	17	-7	16	17	1	-8	52	56	3	5	60	58	6	-14	23	24
5	-3	32	29	7	8	35	36	10	-12	11	10	13	-10	34	36	17	-6	20	21	1	-6	44	47	3	6	9	6	6	-13	20	20
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5	0	123	120	7	11	12	12	10	-8	32	32	13	-5	30	28	17	-2	24	21	1	-3	102	107	3	9	25	24	6	-9	29	29
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5	4	28	27	8	-11	12	14	10	-3	36	36	13	-1	34	37	17	4	16	15	1	2	41	43	4	-14	29	31	6	-4	27	24
5	10	40	45	8	-10	11	10	10	-2	37	39	13	0	86	87	17	5	17	17	1	3	20	28	4	-13	50	48	6	-3	55	55
5	13	16	18	8	-9	21	22	10	-1	27	26	13	1	16	18	18	-8	15	19	1	4	13	15	4	-12	20	20	6	-2	62	64
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6	-14	34	37	8	-7	90	90	10	1	81	81	13	4	9	7	18	-6	26	26	1	7	81	82	4	-9	28	29	6	0	35	33
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6	-10	14	14	8	-4	34	34	10	6	17	15	13	9	17	18	18	-1	40	38	1	12	19	18	4	-6	69	71	6	4	52	51
6	-9	53	55	8	-3	14	13	10	7	12	16	13	10	22	21	18	1	18	19	2	-16	28	29	4	-5	27	27	6	5	43	46
6	-7	73	75	8	-2	21	20	10	8	47	49	14	-9	12	15	18	2	16	14	2	-15	13	9	4	-4	79	84	6	7	32	30
6	-5	44	45	8	-1	23	23	10	9	10	8	14	-8	39	39	18	3	15	14	2	-14	24	25	4	-3	116	112	6	8	56	56
6	-4	87	81	8	0	46	47	10	10	17	17	14	-7	28	29	18	4	24	27	2	-13	33	34	4	-2	27	24	6	9	24	22
6	-3	52	53	8	1	61	60	10	11	16	15	14	-5	21	23	19	-6	10	8	2	-12	35	35	4	0	25	26	6	10	17	19
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6	0	45	47	8	4	46	46	11	-10	49	50	14	0	21	22	19	-3	30	31	2	-8	29	30	4	3	50	51	7	-15	29	29
6	1	40	40	8	5	13	12	11	-9	10	11	14	1	50	50	19	-2	14	15	2	-7	47	45	4	4	48	47	7	-14	13	13
6	2	49	52	8	8	42	43	11	-8	86	87	14	3	22	21	19	-1	23	22	2	-6	34	38	4	5	36	35	7	-13	25	26
6	3	131	130	8	9	13	13	11	-2	12	11	14	4	27	27	19	0	21	21	2	-5	31	27	4	6	28	31	7	-10	42	42
6	4	103	106	8	10	32	30	11	-1	13	12	14	6	12	13	19	1	16	15	2	-4	116	111	4	7	27	27	7	-9	9	9
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7	-8	33	38	9	-3	33	33	12	-7	12	11	16	-9	10	8	0	-6	20	19	3	-12	31	32	5	-5	7	6	7	6	21	20
7	-7	72	75	9	-2	27	30	12	-5	72	72	16	-8	37	37	0	-4	109	110	3	-11	63	65	5	-4	41	40	7	7	49	51
7	-6	10	13	9	-1	18	22	12	-4	9	11	16	-7	27	28	0	-2	63	63	3	-10	11	10	5	-3	63	64	7	8	39	40
7	-5	23	21	9	0	91	90	12	-3	16	16	16	-6	58	60	0	0	20	20	3	-9	82	84	5	-2	60	61	7	9	25	25
7	-4	66	65	9	1	65	65	12	-2	15	16	16	-1	17	14	0	2	62	61	3	-8	95	93	5	-1	55	54	7	10	39	38
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7	-2	48	48	9	4	59	59	12	0	54	56	16	2	22	21	0	6	121	122	3	-6	32	37	5	1	7	9	8	-13	13	13
7	-1	42	41	9	5	17	19	12	1	63	63	16	3	29	30	0	8	21	19	3	-5	19	19	5	2	32	32	8	-8	20	20
7	0	0	6	9	6	44	43	12	2	33	29	16	4	39	38	0	10	10	12	3	-4	150	153	5	3	82	82	8	-7	21	22
7	1	29	31	9	7	20	18	12	5	51	49	16	5	10	8	0	12	17	21	3	-3	26	21	5	4	32	31	8	-6	30	29
7	2	9	11	9	8	11	12	12	6	10	10	16	6	11	9	1	-16	13	9	3	-2	74	72	5	5	24	23	8	-5	69	70

Table A-5. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
8	-3	22	22	11	-5	21	21	14	4	53	52	0	2	40	40	3	-9	47	49	5	0	27	28	8	-3	36	36	11	1	8	3
8	-2	24	24	11	-4	80	79	14	5	33	32	0	4	7	2	3	-8	74	74	5	1	16	17	8	-2	64	65	11	2	37	37
8	-1	34	31	11	-3	24	25	14	7	16	17	0	6	36	39	3	-7	66	66	5	2	36	37	8	-1	86	85	11	4	13	14
8	0	40	39	11	-2	28	29	14	8	21	22	0	8	12	12	3	-6	27	24	5	3	44	43	8	0	59	60	11	6	51	52
8	1	36	37	11	-1	27	27	15	-11	15	14	0	10	31	30	3	-5	51	49	5	4	64	66	8	1	13	14	11	8	35	32
8	2	21	20	11	0	75	75	15	-7	22	22	1	-15	22	21	3	-4	87	82	5	8	10	11	8	2	11	9	11	9	10	3
8	3	55	56	11	1	26	25	15	-2	20	21	1	-14	10	6	3	-3	34	36	5	10	35	34	8	4	25	26	12	-11	31	33
8	4	84	84	11	2	98	99	15	-1	34	36	1	-12	29	28	3	-2	32	32	6	-15	11	5	8	5	25	26	12	-7	23	19
8	5	72	72	11	3	15	14	15	0	18	21	1	-11	47	48	3	-1	28	32	6	-14	15	15	8	7	59	58	12	-6	13	15
8	6	27	28	11	4	13	12	15	2	13	12	1	-10	18	18	3	0	22	23	6	-13	28	29	8	10	13	9	12	-5	25	24
8	8	25	28	11	5	12	13	15	3	53	53	1	-9	94	96	3	1	55	57	6	-12	16	17	9	-14	12	13	12	-3	21	22
8	8	58	59	11	7	14	14	15	4	15	13	1	-8	34	32	3	2	23	21	6	-9	51	50	9	-12	11	9	12	-2	35	35
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8	11	11	7	11	9	12	7	16	-9	16	18	1	-6	50	55	3	4	53	55	6	-7	39	38	9	-9	25	25	12	0	12	10
9	-14	22	21	12	-11	40	40	16	-8	25	26	1	-5	148	147	3	7	12	11	6	-6	65	65	9	-8	35	35	12	1	38	34
9	-11	11	11	12	-9	31	32	16	-7	13	16	1	-4	10	17	3	8	43	43	6	-4	7	12	9	-7	49	47	12	2	11	18
9	-10	84	84	12	-8	16	17	16	-6	42	41	1	-3	82	82	3	9	18	17	6	-3	36	36	9	-6	31	29	12	3	29	32
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9	-7	34	31	12	-5	59	60	16	-4	13	13	1	-1	14	13	3	11	22	23	6	-1	71	71	9	-3	37	36	12	7	36	36
9	-6	45	45	12	-4	16	15	16	-3	30	32	1	0	31	30	4	-15	13	11	6	0	10	11	9	-2	19	19	12	8	13	12
9	-5	48	47	12	-3	24	22	16	-2	54	53	1	1	61	62	4	-14	14	14	6	1	34	37	9	-1	42	42	13	-12	10	9
9	-4	55	55	12	-1	82	82	16	0	25	25	1	2	12	11	4	-13	39	40	6	2	34	35	9	0	28	27	13	-10	15	14
9	-3	15	15	12	0	17	18	16	1	37	39	1	4	21	21	4	-12	34	33	6	3	15	16	9	1	14	12	13	-9	16	15
9	-2	16	14	12	1	42	42	16	5	22	22	1	5	36	37	4	-11	21	21	6	4	53	54	9	2	65	65	13	-8	12	12
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9	1	32	32	12	3	30	32	17	-8	28	27	1	8	22	23	4	-8	11	12	6	8	21	23	9	5	17	20	13	-5	12	9
9	2	80	81	12	4	24	26	17	-7	16	18	1	9	11	8	4	-7	26	27	6	9	40	40	9	6	44	44	13	-4	11	9
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9	6	15	17	12	7	46	46	17	-5	16	14	1	11	14	13	4	-5	29	26	7	-15	11	11	9	8	11	15	13	-1	26	27
9	7	55	54	12	8	15	15	17	-4	17	19	2	-15	14	16	4	-4	80	80	7	-13	27	25	9	8	14	15	13	0	17	18
9	8	36	36	13	-11	14	14	17	-1	23	23	2	-14	24	24	4	-3	68	69	7	-11	23	24	9	9	12	8	13	1	13	9
9	9	21	20	13	-10	34	35	17	1	13	11	2	-13	35	35	4	-2	64	66	7	-9	18	20	10	-14	15	13	13	2	47	47
9	10	20	21	13	-9	14	14	17	2	16	18	2	-12	42	39	4	-1	58	59	7	-8	68	68	10	-13	14	8	13	3	34	33
9	11	15	14	13	-8	24	26	17	3	43	42	2	-10	54	54	4	0	24	21	7	-7	55	55	10	-12	12	10	13	4	10	18
10	-14	14	13	13	-6	21	20	18	-7	22	25	2	-8	11	11	4	2	44	43	7	-6	29	30	10	-11	50	50	13	6	30	31
10	-11	52	52	13	-3	9	7	18	-6	26	28	2	-7	30	31	4	3	10	10	7	-5	51	51	10	-9	26	24	14	-11	24	24
10	-9	37	36	13	-1	72	73	18	-5	11	16	2	-5	24	22	4	5	58	58	7	-3	52	52	10	-8	51	53	14	-8	23	25
10	-8	14	12	13	0	72	72	18	-4	31	29	2	-4	149	149	4	6	29	29	7	-2	26	24	10	-3	48	49	14	-4	11	8
10	-6	18	21	13	2	21	23	18	-3	38	38	2	-3	45	48	4	7	25	28	7	-1	80	80	10	-2	37	36	14	-3	25	25
10	-5	84	86	13	3	21	22	18	-2	11	10	2	-2	24	25	4	8	24	23	7	1	31	30	10	-1	77	79	14	-2	56	56
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10	3	36	36	14	-6	24	26					2	6	40	39	5	-10	23	22	7	10	22	23	11	-12	17	19	15	-8	11	13
10	4	39	41	14	-5	53	54					2	8	19	18	5	-9	19	16	8	-13	24	22	11	-10	59	59	15	-7	31	32
10	5	17	17	14	-4	40	41	0	-14	23	22	2	9	26	26	5	-8	55	56	8	-12	17	16	11	-9	10	11	15	-6	19	18
10	6	12	15	14	-3	16	16	0	-12	32	34	2	11	27	25	5	-7	74	78	8	-11	49	51	11	-8	24	22	15	-4	10	5
10	7	48	47	14	-2	25	26	0	-10	62	62	3	-16	11	14	5	-6	21	22	8	-10	15	15	11	-4	27	26	15	-3	45	45
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11	-9	13	8	14	0	29	29	0	-6	156	154	3	-14	29	29	5	-3	12	8	8	-6	63	62	11	-2	29	27	15	2	23	25
11	-8	19	20	14	2	19	19	0	-2	21	23	3	-13	21	20	5	-2	9	6	8	-5	16	20	11	-1	8	3	15	3	43	44
11	-6	73	72	14	3	36	37	0	0	126	130	3	-12	38	39	5	-1	85	87	8	-4	51	52	11	0	45	45	15	4	17	18

Table A-5. (Continued)

K	L	FO	FC
15	5	10	13
16	-9	17	13
16	-8	20	22
16	-6	47	46
16	-4	13	13
16	-2	28	28
16	2	15	16
16	3	15	15
16	4	32	31
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17	-7	23	21
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17	-5	14	16
17	-1	27	26
17	0	12	7
17	1	10	11
17	3	40	40
17	4	16	19
18	-6	15	18
18	-5	10	9
18	-4	15	17
18	-2	20	19
18	-1	11	9
18	1	11	11
18	2	14	10
19	-4	14	12
	H=	5	
3	-16	35	33
3	-14	38	31
3	-10	72	74
3	-8	23	24
3	-6	83	82
3	-4	68	74
3	-2	26	29
3	0	64	63
3	2	39	40
3	4	10	11
3	9	38	37
1	-15	50	48
1	-14	21	19
1	-13	20	20
1	-12	16	17
1	-11	33	32
1	-10	23	21
1	-9	60	59
1	-8	13	11
1	-7	10	9
1	-6	41	41
1	-5	81	85
1	-4	10	14
1	-3	15	17
1	-2	25	27
1	0	3	15
1	1	81	83

K	L	FO	FC
1	2	15	18
1	3	41	41
1	4	40	40
1	5	12	10
1	8	8	6
1	7	27	28
1	9	19	18
1	10	10	3
2	-14	23	24
2	-12	11	3
2	-10	50	51
2	-9	23	20
2	-8	23	27
2	-6	26	29
2	-5	33	34
2	-4	86	85
2	-3	47	48
2	-2	24	24
2	-1	60	61
2	0	89	90
2	1	20	20
2	2	34	36
2	3	30	30
2	4	9	10
2	5	8	7
2	7	26	27
2	8	32	30
2	9	30	31
3	-15	31	30
3	-14	15	19
3	-12	11	12
3	-11	18	17
3	-10	17	20
3	-8	27	28
3	-7	23	20
3	-6	71	71
3	-5	111	108
3	-4	21	18
3	-3	19	19
3	-2	66	64
3	0	69	67
3	2	36	36
3	3	37	39
3	4	54	55
3	5	25	25
3	8	21	20
3	10	21	21
4	-15	17	19
4	-14	12	6
4	-13	21	20
4	-10	34	32
4	-8	55	55
4	-6	22	22
4	-5	29	29
4	-4	37	37
4	-3	14	16

K	L	FO	FC
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4	0	54	55
4	1	41	41
4	2	28	30
4	3	63	64
4	4	18	18
4	5	17	15
4	6	11	14
4	8	11	11
4	9	17	19
4	10	22	20
5	-14	14	13
5	-13	28	27
5	-9	13	14
5	-8	55	56
5	-7	68	70
5	-6	63	63
5	-5	22	26
5	-4	24	24
5	-3	30	30
5	-2	95	98
5	-1	10	15
5	0	56	59
5	1	16	16
5	3	42	41
5	4	26	27
5	5	30	34
5	8	22	22
5	9	15	17
6	-14	20	20
6	-13	21	18
6	-12	33	35
6	-11	17	17
6	-10	10	9
6	-8	48	49
6	-7	19	20
6	-6	13	16
6	-5	29	30
6	-4	12	12
6	-3	23	20
6	-2	60	58
6	-1	65	64
6	0	26	27
6	1	13	14
6	2	23	22
6	3	37	38
6	5	19	20
6	6	50	50
6	9	17	17
7	-14	25	24
7	-13	31	30
7	-12	10	10
7	-11	9	3
7	-9	23	22
7	-8	26	25

K	L	FO	FC
7	-7	51	51
7	-6	32	33
7	-5	31	31
7	-4	23	24
7	-3	45	42
7	-2	16	15
7	-1	15	17
7	0	12	14
7	1	14	17
7	3	11	16
7	4	54	54
7	6	20	21
7	9	21	22
8	-14	20	23
8	-13	18	16
8	-12	28	27
8	-11	32	31
8	-10	22	22
8	-9	33	32
8	-8	47	48
8	-7	9	8
8	-4	36	36
8	-3	27	28
8	-2	46	45
8	-1	41	41
8	0	25	22
8	1	49	49
8	3	19	17
8	6	24	23
8	7	20	19
8	9	24	23
9	-13	32	32
9	-12	19	20
9	-11	38	36
9	-10	18	20
9	-9	25	25
9	-6	27	29
9	-7	11	13
9	-4	55	54
9	-3	25	24
9	-2	15	15
9	-1	42	42
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9	6	39	39
9	7	15	15
10	-13	14	11
10	-11	44	44
10	-10	13	11
10	-9	19	20
10	-8	20	20
10	-7	12	12
10	-5	31	32

K	L	FO	FC
10	-4	41	39
10	-1	60	60
10	-2	8	1
10	-1	20	21
10	0	22	22
10	1	43	48
10	2	26	28
10	3	13	10
10	5	22	22
10	7	35	34
11	-12	21	20
11	-10	10	9
11	-8	47	46
11	-5	9	10
11	-4	47	48
11	-2	16	14
11	0	12	11
11	1	9	9
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12	1	42	44
12	2	10	9
12	5	13	15
12	7	40	39
13	-12	14	11
13	-11	23	23
13	-9	11	15
13	-5	18	18
13	-4	14	12
13	-3	23	23
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13	-1	21	18
13	0	13	11
13	2	29	29
13	3	20	16
13	5	23	21
13	6	27	29
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14	-6	24	23
14	-4	15	16
14	-2	25	24
14	-1	11	9
14	1	32	34
15	-8	11	7
15	-7	36	34

K	L	FO	FC
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15	-4	10	6
15	-3	30	28
15	-1	12	8
15	1	15	15
15	3	20	21
15	4	18	17
16	-9	14	14
16	-8	26	25
16	-5	13	11
16	-2	23	24
16	-1	16	17
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17	-3	14	17
17	-2	25	25
18	-4	10	10
18	-2	14	12
18	-1	15	13
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0	-10	54	55
0	-8	17	19
0	-6	8	10
0	-4	24	25
0	-2	68	69
0	0	69	69
0	2	77	78
0	4	14	13
0	6	37	36
0	8	46	46
1	-15	54	53
1	-14	10	7
1	-12	28	25
1	-11	26	27
1	-10	24	24
1	-8	3	8
1	-6	8	3
1	-5	56	57
1	-3	49	48
1	-2	42	44
1	-1	11	11
1	0	35	37
1	1	36	36
1	3	46	45
1	6	15	12
1	7	36	35
2	-14	17	19
2	-13	12	9
2	-11	33	34

K	L	FO	FC
2	-10	41	41
2	-9	32	33
2	-8	14	17
2	-7	44	43
2	-6	48	47
2	-5	30	29
2	-4	12	8
2	-2	53	50
2	-1	55	53
2	0	39	39
2	1	12	12
2	2	83	84
2	3	49	44
2	4	9	5
2	7	13	6
2	8	28	26
3	-15	24	24
3	-12	32	34
3	-11	25	27
3	-10	38	38
3	-9	20	19
3	-7	28	26
3	-6	48	47
3	-5	19	17
3	-4	29	30
3	-3	72	71
3	-2	68	68
3	-1	24	22
3	0	43	44
3	2	22	23
3	3	28	28
3	4	15	17
3	6	15	13
3	7	32	32
4	-14	9	0
4	-13	18	21
4	-11	38	38
4	-8	45	46
4	-7	38	38
4	-6	21	21
4	-5	34	35
4	-4	8	4
4	-3	44	44
4	-2	10	8
4	-1	100	100
4	0	22	22
4	2	61	63
4	3	31	30
4	4	19	18
4	6	20	19
5	-14	13	11
5	-13	22	22
5	-12	26	26
5	-10	21	19
5	-9	14	13
5	-7	37	38

K	L	FO	FC
5	-6	69	69
5	-5	47	48
5	-3	10	9
5	-2	34	34
5	-1	43	44
5	0	16	16
5	2	28	29
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6	-13	17	14
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6	-2	37	37
6	-1	61	61
6	0	58	58
6	1	9	6
6	3	23	26
6	4	20	23
7	-14	20	18
7	-13	33	38
7	-12	35	36
7	-11	29	28
7	-9	34	33
7	-8	22	23
7	-6	30	30
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7	-2	37	36
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8	-10	19	18
8	-9	20	20
8	-8	26	24
8	-7	35	32
8	-6	24	27
8	-5	29	29
8	-4	23	24
8	-3	52	48

Table A-5. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
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0	-1	11	12	13	-10	20	18	2	-8	25	25	5	3	12	10	9	5	11	8	0	4	13	14	5	0	29	28	10	-3	17	15
0	0	24	24	13	-8	19	22	2	-6	45	44	5	5	20	19	10	-11	16	16	1	-13	29	29	5	1	10	5	10	-2	10	11
0	1	29	29	13	-7	17	16	2	-5	24	23	5	6	36	32	10	-9	42	42	1	-12	13	15	5	2	11	14	10	-1	16	14
0	2	31	29	13	-6	36	37	2	-2	13	13	6	-13	27	26	10	-8	20	18	1	-11	10	10	5	3	12	13	10	1	12	11
0	3	33	33	13	-5	15	15	2	-1	34	36	6	-12	11	2	10	-5	46	46	1	-10	13	14	6	-13	17	20	11	-9	14	12
0	4	26	28	13	-1	17	16	2	0	9	10	6	-11	20	18	10	-1	10	8	1	-9	62	63	6	-12	12	11	11	-2	33	32
0	5	13	11	13	0	22	22	2	1	9	9	6	-8	18	17	10	-1	9	8	1	-7	30	30	6	-10	32	34	11	-1	10	7
0	6	16	17	13	1	22	23	2	2	50	50	6	-7	51	51	10	1	12	10	1	-8	14	13	6	-8	23	22	12	-6	12	14
0	-13	27	26	14	-9	27	27	2	3	11	8	6	-6	41	40	10	2	27	25	1	-5	17	17	6	-7	24	22	12	-5	21	22
0	-12	18	18	14	-8	30	30	2	5	27	26	6	-5	16	18	10	3	26	26	1	-4	14	11	6	-6	35	34	12	-3	21	22
0	-11	9	11	14	-6	29	30	2	6	28	30	6	-4	12	9	11	-10	34	34	1	-3	28	27	6	-5	28	28	12	-2	12	14
0	-10	16	11	14	-7	13	11	2	7	12	5	6	-2	49	51	11	-8	19	20	1	1	26	27	6	-3	12	11	12	-1	12	10
0	-8	42	41	14	-5	13	14	3	-14	11	8	6	0	18	19	11	-6	25	24	1	4	11	11	6	-2	14	16	13	+5	12	10
0	-6	11	9	14	-4	11	11	3	-13	14	13	6	1	19	17	11	-4	43	44	2	-14	24	20	6	0	13	10				
0	-5	52	53	14	-3	15	16	3	-12	43	45	6	2	10	9	11	-3	15	12	2	-13	14	15	6	1	14	13		H=	9	
0	-3	15	18	14	0	23	24	3	-11	18	17	6	3	18	18	11	-2	27	27	2	-11	10	6	6	2	12	10				
0	-2	15	14	14	1	21	19	3	-10	26	28	6	4	34	34	11	2	13	14	2	-10	24	25	6	3	13	9	0	-10	30	29
0	-1	15	19	14	3	18	17	3	-9	30	33	6	5	23	22	12	-10	14	16	2	-9	12	11	6	4	16	16	0	-8	38	39
0	0	11	14	15	-9	14	14	3	-8	30	30	6	6	13	9	12	-9	33	34	2	-8	44	44	7	-12	19	20	0	-6	13	14
0	1	38	38	15	-8	15	14	3	-7	15	16	7	-13	10	12	12	-8	10	7	2	-7	14	15	7	-11	26	29	0	-4	36	34
0	2	29	27	15	-7	15	17	3	-6	30	31	7	-12	28	29	12	-5	35	35	2	-6	17	15	7	-10	16	16	0	-2	24	22
0	3	24	26	15	-5	22	21	3	-5	21	19	7	-11	11	11	12	-4	9	6	2	-4	25	29	7	-9	17	17	1	-9	51	50
0	5	17	19	15	-2	17	18	3	-2	26	27	7	-10	22	18	12	-2	11	9	2	-1	21	18	7	-8	18	19	1	-6	12	11
0	6	33	32	15	-1	17	18	3	-1	30	30	7	-9	16	16	12	0	21	19	2	0	12	10	7	-7	27	27	1	-5	21	23
0	-13	22	19	15	1	14	13	3	0	12	12	7	-8	16	14	12	1	14	12	2	1	30	30	7	-6	13	12	1	-3	18	16
0	-11	13	12	16	-7	13	19	3	1	37	39	7	-6	22	21	12	3	20	18	2	2	23	21	7	-5	32	32	1	-1	17	15
0	-10	20	20	16	0	31	30	3	3	22	21	7	-4	19	18	13	-9	14	14	2	3	11	10	7	-4	14	12	1	2	10	8
0	-9	49	50					3	6	22	20	7	-2	25	27	13	-8	14	11	2	5	15	17	7	-3	26	27	2	-12	10	7
0	-8	25	24		H=	7		4	-14	11	10	7	-1	37	38	13	-6	11	11	3	-13	23	20	7	-1	30	28	2	-10	19	21
0	-5	33	35					4	-13	34	34	7	0	19	19	13	-5	20	21	3	-12	29	28	7	0	20	18	2	-8	17	16
0	-3	37	39	0	-10	19	19	4	-11	43	39	7	1	34	33	13	-4	22	22	3	-11	17	14	7	2	18	17	2	-5	34	31
0	-1	8	8	0	-8	39	39	4	-10	18	17	7	3	40	38	13	-3	13	9	3	-10	13	16	8	-12	15	13	2	-4	27	26
0	0	9	7	0	-6	21	22	4	-9	33	36	7	5	22	22	13	-2	22	21	3	-9	26	27	8	-11	14	13	2	-3	14	12
0	1	47	47	0	-2	21	20	4	-8	19	18	8	-10	14	11	13	-1	23	23	3	-8	15	14	8	-10	27	27	2	-2	16	14
0	3	9	5	0	0	38	38	4	-7	60	61	8	-9	31	32	13	0	16	16	3	-3	19	21	8	-9	10	8	2	1	13	8
0	4	12	10	0	2	73	75	4	-6	13	14	8	-7	20	20	13	1	10	8	3	0	15	16	8	-6	23	22	2	2	11	9
0	5	24	23	0	6	26	26	4	-4	21	20	8	-6	33	32	13	2	11	9	3	1	15	15	8	-7	26	25	3	-11	17	15
0	6	11	9	1	-15	29	30	4	-2	31	31	8	-5	46	43	14	-8	11	10	3	2	24	24	8	-6	35	35	3	-10	14	14
0	-10	19	20	1	-13	27	28	4	0	32	28	8	-3	12	13	14	-6	25	26	3	4	18	19	8	-5	23	23	3	-9	36	35
0	-9	22	22	1	-12	14	13	4	1	14	16	8	-2	41	41	14	-5	20	22	4	-13	30	28	8	-4	16	16	3	-6	36	37
0	-5	21	18	1	-11	25	27	4	2	18	18	8	-1	28	26	14	-3	13	12	4	-11	17	14	8	-2	25	26	3	-4	15	15
0	-4	64	63	1	-9	32	32	4	3	12	13	8	0	22	24	14	-2	16	17	4	-9	12	14	8	-1	13	9	3	-4	17	15
0	-2	14	14	1	-8	14	14	4	4	27	26	8	2	26	26	14	0	29	28	4	-8	17	17	8	3	22	22	3	-2	14	15
0	0	32	33	1	-6	26	24	4	5	16	16	8	3	19	20	15	-6	14	14	4	-6	10	11	9	-11	13	16	3	-1	23	19
0	1	12	10	1	-5	10	7	4	6	12	14	8	4	27	28	15	-5	28	27	4	-5	37	36	9	-10	16	17	3	0	21	21
0	2	16	16	1	-3	76	77	5	-14	10	8	8	5	30	27	15	-2	11	8	4	-2	18	19	9	-9	28	24	3	1	11	10
0	-12	17	17	1	-2	11	13	5	-13	13	14	9	-10	38	39					4	1	25	23	9	-7	26	25	4	-12	11	12
0	-11	15	13	1	0	12	9	5	-12	64	64	9	-5	11	11		H=	8		4	2	18	17	9	-6	16	15	4	-11	12	11
0	-9	48	49	1	1	55	57	5	-11	12	10	9	-4	40	41					4	4	11	8	9	-5	19	20	4	-9	18	15
0	-8	19	17	1	3	20	17	5	-10	22	23	9	-3	20	23	0	-14	36	35	5	-12	21	22	9	-4	20	18	4	-7	13	15
0	-7	11	11	1	4	11	5	5	-9	28	38	9	-2	13	12	0	-10	23	24	5	-11	20	24	9	-3	10	8	4	-6	17	17
0	-5	40	33	1	7	41	39	5	-8	12	13	9	-1	24	21	0	-8	33	35	5	-10	14	11	9	-2	27	25	4	-5	35	35
0	-3	28	29	2	-13	30	31	5	-5	21	22	9	0	18	20	0	-6	15	15	5	-8	19	21	9	1	11	7	4	-4	12	12
0	-1	9	11	2	-11	34	34	5	-4	12	14	9	1	17	18	0	-4	52	52	5	-7	13	15	9	2	32	31	4	-3	11	8
0	1	35	34	2	-10	11	8	5	-2	41	39	9	3	17	17	0	-2	8	7	5	-5	11	15	10	-5	26	26	4	-1	21	22

Table A-5. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FC	FC	K	L	FO	FC
4	1	13	17	4	-3	16	14								
5	-11	22	23	5	-5	31	29								
5	-10	15	15	5	-5	15	14								
5	-7	25	24												
5	-6	41	43												
5	-5	15	18												
5	-4	23	20												
5	-2	16	16												
5	-1	13	12												
5	1	25	23												
5	1	11	10												
6	-11	13	11												
6	-6	14	20												
6	-5	33	29												
6	-2	20	18												
6	-1	27	25												
7	-12	21	19												
7	-6	14	17												
7	-7	27	29												
7	-6	17	15												
7	-5	15	12												
7	1	25	21												
8	-10	14	13												
8	-8	11	10												
8	-6	13	13												
8	-6	23	22												
8	-5	14	16												
8	-3	15	14												
8	-3	22	20												
9	-6	14	13												
9	-2	23	21												
10	-7	15	16												
10	-3	23	21												
	-4	11													
0	-8	12	12												
0	-2	33	35												
1	-9	20	19												
1	-7	20	19												
1	-6	16	15												
1	-5	17	15												
1	-3	17	16												
1	-2	12	10												
2	-9	13	11												
2	-7	11	19												
2	-5	21	20												
2	-4	10	9												
2	-2	31	29												
3	-9	15	14												
3	-7	23	20												
3	-6	37	34												
3	-4	14	14												
4	-7	15	15												
4	-5	29	26												
4	-4	13	11												

Table A-6. Observed (FO) and Calculated (FC) Structure Factors for $[CuPIPA(H_2O)]_2 \cdot 2H_2O$

K	L	FO	FC
	H=-24		
0	12	23	22
0	10	15	14
	H=-23		
1	5	35	36
1	7	20	19
1	11	22	23
1	13	37	35
	H=-22		
0	4	27	26
0	6	37	37
0	8	18	20
0	10	16	17
0	12	29	30
0	14	28	29
0	16	16	15
2	4	25	23
2	5	16	16
2	6	31	31
2	7	18	17
2	8	15	14
2	10	14	14
2	11	17	18
2	12	23	25
2	13	21	17
2	14	28	27
	H=-21		
1	3	15	13
1	5	44	43
1	6	15	13
1	7	36	38
1	11	19	20
1	12	11	14
1	13	46	47
1	14	15	16
1	15	25	26
3	5	28	27
3	6	22	22
3	7	18	19
3	8	19	17
3	12	24	22
3	13	20	23
3	14	24	24
	H=-20		
0	0	25	27
0	4	26	26
0	6	41	41
0	8	32	33
0	12	18	20
0	14	49	49
0	16	33	32
0	18	12	11
2	0	24	23
2	4	21	22
2	5	17	20
2	6	38	37
2	7	19	15
2	8	25	24
2	12	22	21
2	14	42	42
2	15	15	15
2	16	28	27
4	5	25	24
4	6	18	19
4	7	19	20
4	11	17	14
4	12	12	9
4	13	21	21
	H=-19		
1	1	23	23
1	3	15	15
1	4	14	12
1	5	43	44
1	6	16	16
1	7	38	37
1	13	37	39
1	15	30	29
1	16	11	7
1	17	16	19
3	0	13	15
3	2	12	12
3	4	15	15
3	5	22	24
3	6	23	25
3	7	22	21
3	8	15	14
3	12	11	11
3	13	31	31
3	14	25	24
3	15	22	19
3	16	12	11
5	4	14	13
5	6	26	26
5	8	15	17
	H=-18		
0	0	46	47
0	2	17	16
0	4	14	10
0	6	57	58
0	8	22	23
0	12	20	21
0	14	52	51
0	16	23	23
2	0	34	34
2	1	22	19
2	5	14	11
2	6	58	58
2	8	31	32
2	10	18	18
2	13	14	9
2	14	39	40
2	15	16	15
2	16	22	23
4	0	15	15
4	5	29	27
4	6	23	25
4	7	30	28
4	8	13	12
4	10	13	11
4	11	14	6
4	14	18	20
4	15	24	22
	H=-17		
1	2	11	12
1	3	29	28
1	5	19	17
1	7	41	41
1	8	11	11
1	9	25	27
1	11	18	19
1	13	30	30
1	15	31	30
1	16	12	10
1	17	29	32
3	2	17	18
3	5	23	21
3	6	19	20
3	7	32	32
3	8	15	16
3	9	20	20
3	11	14	15
3	13	19	17
3	14	18	19
3	15	17	14
3	16	15	13
3	17	17	18
5	0	13	14
5	2	13	14
5	6	31	32
5	8	21	24
5	14	14	15
	H=-16		
0	0	26	21
0	2	15	14
0	4	26	28
0	6	58	58
0	8	34	35
0	10	17	16
0	14	20	18
0	16	21	22
0	18	23	22
2	0	41	42
2	2	13	10
2	4	34	35
2	5	13	8
2	6	47	48
2	7	16	15
2	8	36	36
2	10	20	21
2	11	15	14
2	14	18	18
2	15	14	11
2	16	20	21
2	18	23	22
4	0	32	31
4	3	16	13
4	4	19	19
4	6	29	30
4	7	20	23
4	8	20	19
4	9	16	16
4	14	22	21
4	15	16	18
4	16	14	13
4	17	23	21
6	6	14	17
6	7	25	25
6	9	17	13
6	10	11	13
	H=-15		
1	1	16	15
1	3	35	37
1	7	31	34
1	8	12	13
1	9	56	59
1	10	13	12
1	11	26	26
1	12	12	13
1	14	11	14
1	17	35	36
1	19	17	16
3	0	12	14
3	1	18	19
3	3	35	38
3	7	21	22
3	8	15	15
3	9	31	32
3	11	14	11
3	13	17	17
3	15	22	24
3	17	33	32
3	18	14	15
5	0	23	24
5	2	17	19
5	3	22	24
5	4	13	12
5	7	21	19
5	8	21	21
5	9	21	20
5	10	17	16
5	11	15	18
	H=-14		
0	0	56	57
0	2	29	30
0	4	20	19
0	6	23	24
0	8	34	35
0	10	25	23
0	12	19	21
0	14	19	20
0	16	17	13
0	18	44	43
0	20	15	13
2	0	44	45
2	1	25	23
2	2	30	31
2	4	32	32
2	5	14	11
2	6	20	20
2	7	20	18
2	8	34	35
2	9	18	18
2	10	37	37
2	12	34	36
2	13	16	14
2	14	14	12
2	16	10	8
2	18	37	37
4	0	14	14
4	1	25	27
4	2	13	10
4	4	23	24
4	5	16	16
4	6	18	18
4	7	23	25
4	8	21	21
4	9	35	36
4	10	23	23
4	11	23	25
4	12	22	23
4	14	19	19
4	16	14	13
6	1	20	19
6	2	11	9
6	3	17	12
6	4	18	19
6	6	12	10
6	7	19	17
6	9	26	27
6	11	18	21
6	12	12	12
	H=-13		
1	0	19	18
1	1	80	83
1	2	32	31
1	3	72	75
1	4	30	29
1	5	14	11
1	6	17	18
1	7	14	17
1	9	64	64
1	10	14	13
1	11	50	50
1	15	30	30
1	17	30	29
1	19	27	29
3	0	21	21
3	1	29	31
3	2	26	27
3	3	27	27
3	4	13	14
3	7	26	25
3	8	16	17
3	9	43	45
3	10	39	39
3	11	46	48
3	14	12	11
3	16	14	15
3	17	19	18
3	18	21	21
5	0	19	19
5	1	14	12
5	2	22	22
5	3	20	18
5	4	12	11
5	8	19	20
5	10	44	44
5	11	18	19
5	12	24	23
7	2	17	17
7	4	12	12
	H=-12		
0	0	29	34
0	2	61	60
0	4	50	49
0	8	40	40
0	10	80	79
0	12	97	95
0	14	49	48
0	16	31	31
0	18	55	54
0	20	27	27
2	0	35	35
2	1	30	30
2	2	63	65
2	3	35	35
2	4	63	63
2	6	15	13
2	7	22	22
2	8	13	15
2	9	27	29
2	10	55	55
2	11	32	34
2	12	79	77
2	14	26	25
2	15	21	19
2	16	10	8
2	18	35	35
2	19	17	18
4	0	17	18
4	1	45	46
4	2	24	23
4	3	51	52
4	4	22	22
4	5	22	22
4	6	13	12
4	7	16	16
4	8	13	12
4	9	24	26
4	10	21	21
4	11	42	43
4	12	34	33
4	14	12	13
6	1	31	29
6	3	23	25
6	7	17	19
6	9	22	19
6	11	27	29
	H=-11		
1	1	80	83
1	2	18	20
1	3	72	71
1	4	23	24
1	5	36	38
1	7	32	32
1	9	42	44
1	10	24	24
1	11	91	94
1	12	29	28
1	13	31	32
1	14	12	12
1	17	30	31
1	19	27	29
3	0	15	14
3	1	54	56
3	2	45	45
3	3	46	50
3	4	41	42
3	5	27	29
3	8	20	20
3	9	22	21
3	10	54	54
3	12	47	46
3	16	30	31
3	17	23	25
3	18	24	25
5	0	16	17
5	2	43	45
5	4	49	50
5	6	13	13
5	10	33	32
5	11	16	16
5	12	32	31
5	16	22	23
7	2	19	19
7	3	15	10
7	4	21	22
7	8	11	11
7	10	24	22
	H=-10		
0	0	28	27
0	2	91	88
0	4	148	144
0	8	54	53
0	10	99	99
0	18	48	48
0	16	13	13
0	12	101	101
0	20	27	26
2	0	10	8
2	1	38	39
2	2	59	59
2	6	19	20
2	3	51	51
2	5	12	7
2	4	116	113
2	7	20	18

Table A-6. (Continued)

K	L	FO	FC
2	8	11	14
2	9	23	24
2	10	56	55
2	11	31	31
2	12	67	66
2	13	32	34
2	16	11	8
2	17	14	14
2	18	35	35
2	19	17	15
4	1	31	32
4	2	18	20
4	3	60	59
4	4	39	38
4	5	27	28
4	9	15	13
4	10	28	27
4	11	31	32
4	12	26	30
4	13	31	31
4	14	10	9
4	17	19	20
6	1	20	18
6	3	36	36
6	5	18	16
6	9	17	13
6	11	30	28
6	13	20	19
	H=	-9	
1	1	59	60
1	2	27	28
1	3	80	80
1	4	48	47
1	5	106	109
1	6	39	37
1	9	35	36
1	11	62	63
1	13	42	42
1	15	18	18
1	16	10	9
1	17	35	34
1	19	34	35
3	0	15	14
3	1	39	40
3	2	61	62
3	3	29	30
3	4	68	67
3	5	42	42
3	6	24	24
3	7	12	11
3	8	41	40
3	9	31	33
3	10	47	47
3	11	46	48

K	L	FO	FC
3	12	38	39
3	13	33	33
3	14	14	13
3	16	16	17
3	17	15	18
3	18	20	21
5	2	37	37
5	4	45	45
5	5	18	18
5	6	17	17
5	8	20	21
5	10	32	32
5	11	12	10
5	12	30	30
5	14	14	12
5	16	12	11
7	2	24	22
7	4	25	25
7	6	13	11
7	10	16	16
	H=	-8	
0	0	19	18
0	2	105	103
0	4	175	173
0	8	16	17
0	10	86	87
0	12	60	58
0	14	25	25
0	18	40	41
2	2	49	49
2	3	32	31
2	4	109	108
2	5	46	45
2	6	20	22
2	7	27	29
2	9	15	14
2	10	44	42
2	11	32	32
2	12	38	37
2	13	26	26
2	14	15	14
2	16	9	6
2	18	26	26
2	19	22	20
4	3	34	34
4	4	46	46
4	5	38	39
4	7	26	26
4	8	9	6
4	10	26	26
4	11	33	33
4	12	33	32
4	13	28	29
4	14	12	10

K	L	FO	FC
4	16	11	10
6	1	14	13
6	3	35	36
6	4	10	9
6	5	21	20
6	9	20	18
6	11	29	29
6	13	25	24
8	0	12	5
8	3	20	19
8	5	16	12
	H=	-7	
1	0	18	17
1	1	13	13
1	2	18	18
1	3	31	33
1	4	17	17
1	5	73	78
1	7	57	59
1	9	17	16
1	11	39	39
1	13	61	62
1	15	19	21
1	19	31	34
3	0	9	7
3	1	34	33
3	2	40	40
3	3	54	53
3	4	28	28
3	5	68	70
3	6	34	35
3	7	22	23
3	8	9	9
3	9	20	19
3	10	17	17
3	11	33	35
3	12	29	29
3	13	42	43
3	14	15	15
3	16	10	10
3	18	11	10
5	0	11	11
5	2	35	35
5	3	20	19
5	4	28	29
5	5	22	24
5	6	31	31
5	8	11	10
5	10	15	15
5	12	19	21
5	13	15	13
5	14	10	10
7	2	28	28
7	4	23	23

K	L	FO	FC
7	6	23	23
7	10	13	13
7	12	21	18
	H=	-6	
0	4	73	73
0	8	47	45
0	12	44	43
0	14	39	39
0	16	33	33
2	0	51	51
2	2	33	34
2	3	22	22
2	4	44	43
2	5	22	26
2	6	10	5
2	7	15	17
2	8	34	35
2	10	11	8
2	11	17	18
2	12	32	32
2	14	20	20
2	15	14	12
2	16	18	18
2	18	13	14
4	0	32	32
4	1	28	27
4	2	32	32
4	3	15	18
4	4	58	60
4	5	27	29
4	6	31	30
4	7	22	23
4	8	23	23
4	10	20	21
4	11	23	24
4	12	37	37
4	13	14	15
4	15	14	9
4	16	14	14
6	0	18	19
6	3	34	34
6	4	17	17
6	5	42	44
6	6	15	14
6	7	27	27
6	11	29	28
6	12	17	15
6	13	25	23
8	3	15	14
8	5	19	21
	H=	-5	
1	0	22	23

K	L	FO	FC
1	2	20	22
1	3	18	24
1	5	64	68
1	6	28	27
1	7	45	47
1	8	14	15
1	11	20	19
1	12	9	6
1	13	48	50
1	17	17	16
1	19	15	14
3	2	19	19
3	3	41	42
3	4	16	19
3	5	70	72
3	6	24	24
3	7	57	59
3	11	19	21
3	12	13	11
3	13	43	44
3	14	17	17
3	15	18	15
3	16	19	19
3	17	14	12
5	0	13	13
5	4	11	16
5	5	21	20
5	6	39	38
5	7	25	27
5	12	19	18
5	13	19	21
5	14	16	18
7	0	16	18
7	4	16	15
7	6	34	34
	H=	-4	
0	4	22	23
0	8	93	92
0	10	12	8
0	12	43	43
0	14	36	36
0	16	42	41
2	0	39	40
2	1	34	35
2	2	19	19
2	3	17	18
2	4	9	6
2	5	39	41
2	6	36	38
2	7	11	10
2	8	75	74
2	9	14	9
2	11	18	18
2	12	26	27

K	L	FO	FC
2	14	23	23
2	15	15	13
2	16	27	28
4	0	38	38
4	1	23	22
4	2	15	18
4	3	16	14
4	4	30	31
4	5	43	43
4	6	41	41
4	7	26	25
4	8	60	58
4	11	14	14
4	12	17	18
4	14	21	21
4	15	15	16
4	16	25	25
6	0	26	26
6	1	14	13
6	3	15	15
6	5	43	43
6	7	31	32
6	8	12	12
6	9	18	17
6	12	12	10
6	13	15	15
8	1	15	11
8	5	19	15
	H=	-3	
1	0	13	15
1	1	28	31
1	2	10	8
1	4	23	28
1	5	63	67
1	7	100	103
1	8	10	9
1	9	13	15
1	10	8	6
1	12	10	8
1	13	35	36
1	14	12	11
1	15	23	25
1	17	27	27
3	0	23	24
3	1	36	37
3	2	25	24
3	5	43	44
3	6	67	66
3	7	72	72
3	8	55	55
3	9	19	19
3	10	14	14
3	12	14	14
3	13	23	25

K	L	FO	FC
3	14	30	29
3	15	24	22
3	16	13	15
3	17	22	22
5	0	33	33
5	6	40	40
5	7	19	20
5	8	35	35
5	12	17	15
5	13	13	13
5	14	24	25
7	0	21	21
7	2	10	9
7	4	11	10
7	6	27	28
7	8	23	25
	H=	-2	
0	6	146	148
0	8	174	171
0	10	25	24
0	14	25	25
0	16	48	48
2	0	148	147
2	2	21	24
2	3	40	36
2	5	27	27
2	6	61	62
2	7	54	54
2	8	89	85
2	9	37	38
2	11	12	8
2	12	22	22
2	14	34	33
2	15	16	16
2	16	37	38
4	0	97	96
4	1	22	20
4	2	16	17
4	6	37	36
4	7	32	33
4	8	43	44
4	9	25	24
4	11	12	10
4	13	18	17
4	14	18	18
4	15	27	27
4	16	22	22
6	0	17	15
6	1	28	30
6	2	12	12
6	5	14	14
6	7	37	37
6	9	30	27
6	13	14	9

K	L	FO	FC
8	7	18	19
	H=	-1	
1	2	7	6
1	3	53	55
1	5	22	26
1	6	14	16
1	7	88	89
1	8	21	19
1	9	58	59
1	11	26	24
1	12	12	13
1	13	29	32
1	14	12	12
1	15	38	40
1	17	32	32
3	0	113	112
3	1	69	70
3	2	35	37
3	4	23	22
3	5	15	17
3	6	54	54
3	7	62	61
3	8	73	72
3	9	38	38
3	10	25	24
3	11	20	20
3	12	13	13
3	13	24	23
3	14	24	24
3	15	25	25
3	16	14	14
5	0	62	62
5	1	16	16
5	2	26	28
5	6	31	32
5	7	18	17
5	8	52	51
5	10	13	10
5	12	16	16
5	14	25	26
7	0	33	33
7	2	20	19
7	6	18	18
7	8	31	32
7	10	14	11
	H=	0	
0	4	19	19
0	6	87	86
0	8	108	104
0	10	37	37
0	14	46	45
0	16	40	39

Table A-6. (Continued)

K	L	FO	FC
2	1	134	132
2	3	42	41
2	4	26	27
2	6	72	72
2	7	38	36
2	8	79	76
2	9	36	34
2	10	25	25
2	13	24	23
2	14	35	36
2	15	18	16
2	16	29	30
2	17	18	16
4	0	73	72
4	1	47	47
4	2	16	17
4	3	16	16
4	4	9	7
4	5	19	18
4	6	24	23
4	7	52	54
4	8	41	41
4	9	45	47
4	11	15	13
4	12	14	13
4	13	20	22
4	15	23	22
6	0	16	15
6	1	38	38
6	2	11	7
6	4	21	21
6	7	36	36
6	9	33	33
6	11	18	18
8	1	19	18
8	2	11	8
8	7	17	13

H= 1

K	L	FO	FC
1	2	42	43
1	3	72	71
1	4	24	26
1	5	24	22
1	6	27	26
1	7	63	64
1	8	17	16
1	9	90	90
1	11	38	39
1	12	15	16
1	13	34	34
1	14	17	18
1	15	44	45
1	16	13	13
3	0	114	112
3	1	81	79

K	L	FO	FC
3	2	106	106
3	3	23	24
3	4	12	12
3	6	39	38
3	7	36	38
3	8	48	47
3	9	52	54
3	10	34	34
3	11	32	31
3	14	17	18
3	15	16	16
5	0	62	62
5	2	41	40
5	4	23	24
5	6	35	34
5	8	33	34
5	10	25	25
7	0	34	33
7	2	20	20
7	5	15	12
7	6	14	13
7	8	17	14
7	10	12	12

H= 2

K	L	FO	FC
0	4	42	42
0	6	39	39
0	8	83	82
0	10	54	54
0	12	39	41
0	14	27	25
0	16	25	25
2	0	146	147
2	1	60	58
2	2	17	17
2	3	37	36
2	4	15	16
2	6	35	35
2	7	43	42
2	8	61	60
2	9	35	36
2	10	26	26
2	11	29	29
2	12	18	18
2	14	27	27
2	15	19	16
2	16	26	27
4	0	96	96
4	1	78	77
4	2	24	23
4	3	42	42
4	4	26	27
4	7	41	44
4	8	29	31
4	9	25	26

K	L	FO	FC
4	11	25	23
4	13	14	11
6	0	16	15
6	1	56	57
6	2	13	17
6	3	27	30
6	7	30	30
6	8	17	18
6	9	17	15
6	11	15	17
8	1	17	17

H= 3

K	L	FO	FC
1	0	15	15
1	3	102	103
1	4	36	34
1	5	15	12
1	6	27	26
1	7	56	57
1	8	16	14
1	9	65	66
1	10	12	13
1	11	30	29
1	12	13	12
1	15	22	22
1	16	12	8
3	0	24	24
3	1	87	85
3	2	40	40
3	3	79	78
3	4	12	15
3	5	18	18
3	7	25	26
3	8	10	8
3	9	35	36
3	10	17	18
3	12	24	21
3	15	19	19
5	0	34	33
5	1	24	26
5	2	45	45
5	4	12	13
5	6	17	17
5	7	22	20
5	8	15	15
5	9	23	22
5	10	15	16
5	12	10	7
7	0	23	21
7	2	27	28
7	6	15	13
7	8	18	17

K	L	FO	FC
0	4	97	94
0	6	28	28
0	8	49	49
0	12	42	43
2	0	40	40
2	1	57	55
2	2	15	19
2	3	33	34
2	4	42	42
2	5	17	18
2	7	18	18
2	8	66	66
2	12	38	38
4	0	38	38
4	1	33	35
4	2	21	23
4	3	19	22
4	4	40	38
4	7	40	41
4	8	39	39
4	9	16	16
4	10	11	7
4	12	27	27
6	0	26	26
6	1	35	36
6	2	12	12
6	3	30	31
6	4	13	12
6	5	15	15
6	7	21	22
6	8	14	16
6	9	17	17
8	1	23	23
8	3	18	15

H= 5

K	L	FO	FC
1	0	22	23
1	3	54	57
1	4	16	16
1	5	41	40
1	7	31	30
1	9	31	31
1	11	13	10
1	13	19	19
3	1	55	56
3	3	30	30
3	4	43	43
3	5	27	27
3	6	21	19
3	7	23	21
3	9	26	27
3	10	13	10
3	11	22	21

K	L	FO	FC
3	13	18	21
5	0	13	13
5	1	37	36
5	2	13	15
5	3	16	14
5	4	23	24
5	8	24	24
5	10	28	26
5	11	17	17
7	0	17	18
7	2	22	22
7	4	22	22
7	5	14	11
7	6	13	9

H= 6

K	L	FO	FC
0	2	9	12
0	4	73	73
0	6	55	55
0	8	32	31
0	10	11	10
0	12	38	38
2	0	53	51
2	1	13	11
2	2	33	34
2	4	60	61
2	5	20	18
2	6	29	28
2	8	40	40
2	10	17	18
2	12	41	42
4	0	31	32
4	1	23	26
4	2	29	27
4	3	20	16
4	4	41	41
4	5	20	24
4	6	18	16
4	8	14	14
4	9	22	19
4	11	17	15
4	12	27	26
6	0	16	19
6	1	23	24
6	3	22	21
6	4	11	11
6	5	24	25
6	8	13	7
8	1	18	17
8	3	14	15

H= 7

K	L	FO	FC
1	0	18	17
1	1	85	85

K	L	FO	FC
1	3	11	4
1	5	52	52
1	7	15	11
1	8	10	9
1	9	16	15
1	10	16	17
1	11	35	36
1	13	24	24
3	1	50	47
3	3	23	24
3	4	28	27
3	5	49	49
3	6	21	24
3	7	16	12
3	10	14	18
3	11	23	22
5	0	14	11
5	1	27	29
5	2	29	29
5	3	20	19
5	4	39	38
5	5	23	22
5	6	25	24
5	10	20	20
7	2	17	18
7	4	24	26
7	6	15	14

H= 8

K	L	FO	FC
0	2	26	27
0	4	75	73
0	6	33	34
0	10	21	21
0	12	34	35
2	0	34	33
2	2	42	42
2	3	21	20
2	4	74	73
2	6	34	33
2	9	25	24
2	11	13	11
2	12	34	34
4	3	36	36
4	4	36	36
4	5	28	27
4	6	24	24
4	7	17	16
4	10	11	8
4	11	21	18
6	3	23	23
6	4	13	11
6	5	26	26
6	7	18	13

K	L	FO	FC
1	0	9	5
1	1	29	28
1	2	42	41
1	3	45	45
1	4	30	27
1	5	78	75
1	6	16	13
1	7	33	31
1	9	15	13
1	11	31	31
1	12	12	8
3	0	15	14
3	2	38	37
3	4	32	33
3	5	43	42
3	6	20	22
3	7	21	23
3	10	11	10
5	2	29	29
5	4	34	33
5	5	16	16
5	6	25	25
5	9	14	4
7	2	13	11
7	4	16	16

H= 10

K	L	FO	FC
0	2	26	27
0	4	15	13
0	6	41	41
0	10	18	21
2	0	10	8
2	1	14	9
2	2	24	25
2	3	30	28
2	4	71	70
2	5	32	32
2	6	41	41
2	7	17	15
2	8	12	10
2	10	12	13
4	5	41	40
4	6	14	14
4	7	24	22
4	9	17	18
6	3	17	18
6	5	17	18

K	L	FO	FC
1	1	12	7
1	2	19	20
1	3	42	42
1	4	17	18
1	5	67	66
1	6	24	23
1	7	40	43
3	0	15	14
3	2	16	16
3	3	14	14
3	4	14	16
3	5	33	32
3	6	30	30
3	7	18	16
5	0	18	17
5	2	17	18
5	4	18	16
5	5	14	12
5	6	25	26
7	2	13	12

H= 12

K	L	FO	FC
0	4	41	42
0	6	34	34
0	8	23	24
2	0	36	35
2	3	13	13
2	4	40	40
2	5	23	22
2	6	31	31
2	7	15	13
2	8	19	20
4	0	18	18
4	3	20	19
4	4	17	18
4	5	25	27
4	6	12	10
4	7	16	17
6	3	15	13

H= 13

K	L	FO	FC
1	0	20	18
1	1	20	20
1	3	24	24
1	5	32	32
1	7	26	26
3	0	21	21
3	3	20	15
3	5	26	24
3	6	13	14
3	7	18	18
5	0	20	19

Table A-6. (Continued)

K	L	FO	F
5	4	15	15
	H= 14		
0	0	58	57
0	2	20	19
0	4	20	19
0	6	19	18
0	8	16	17
2	0	45	45
2	1	19	18
2	2	13	13
2	4	24	23
2	6	21	22
4	0	15	14
4	4	15	13
4	5	19	20
4	6	12	10
	H= 15		
1	0	11	10
1	1	30	34
1	5	18	17
1	7	20	21
3	0	13	14
3	1	26	26
3	2	14	15
3	4	11	10
3	5	14	10
5	0	25	24
5	1	20	15
5	2	21	18
	H= 16		
0	0	27	21
0	2	19	18
2	0	41	42
2	2	29	29
4	0	32	31
4	1	22	22
4	2	15	14
4	3	15	10
	H= 17		
1	1	30	30
1	3	18	20
3	1	25	24
3	2	13	10
5	0	13	14
	H= 18		
0	0	47	47

K	L	F	FC
0	2	23	25
0	4	14	10
2	0	34	34
2	2	19	20
2	3	14	8
4	0	16	15
4	1	18	14
	H= 19		
1	1	33	32
3	0	15	15
3	1	20	18
	H= 20		
0	0	28	27
2	0	23	23

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